



# Shannon entropy and thermodynamic properties of an inversely quadratic Yukawa potential model

C. A. Onate<sup>a</sup>, I. B. Okon<sup>b</sup>, J. A. Akinpelu<sup>a</sup>, O. O. Ajani<sup>a</sup>, O. A. Adedewe<sup>c,\*</sup>, B. B. Deji-Jinadu<sup>a</sup>

<sup>a</sup>Department of Physics, Bowen University, Iwo, Osun State, Nigeria

<sup>b</sup>Department of Physics, University of Uyo, Uyo, Nigeria

<sup>c</sup>Federal University of Technology, Akure, Ondo State, Nigeria

## Abstract

An inversely quadratic Yukawa potential is an exponential-type potential that has received little attention only in the bound state to the best of our understanding. This study obtained the solution of the Schrödinger equation for an inversely quadratic Yukawa potential via parametric Nikiforov-Uvarov method and supersymmetric approach. Some thermodynamic properties (vibrational enthalpy, vibrational Gibbs free energy and vibrational entropy) for the Inversely quadratic Yukawa potential are examined. The study is also applied to Shannon entropy as the theoretic quantity. The results obtained showed that the energy eigenvalue for the potential goes in the opposite direction with the quantum state and the screening parameter. The Shannon entropy obtained as a function of the potential strength only obeyed the Heisenberg principle at the ground state and excited states. In both cases, it also satisfied Bialynick-Birula, Mycielski inequality. It is noted that the thermal properties studied as a function of the temperature, even though the studied potential is not a molecular potential, the results followed the trend of the molecular potential.

DOI:10.46481/jnsps.2024.2134

**Keywords:** Bound states, Eigensolutions, Wave equation, Entropy, Thermal properties

## Article History :

Received: 13 May 2024

Received in revised form: 28 June 2024

Accepted for publication: 17 July 2024

Published: 20 August 2024

© 2024 The Author(s). Published by the Nigerian Society of Physical Sciences under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

Communicated by: B. J. Falaye

## 1. Introduction

The early quantum mechanics developed the study of bound states through energy levels. This has greatly involved researchers from different areas of sciences, especially in the field of physical sciences. At first, the study focuses on the analytic solutions for a few potential systems such as the harmonic oscillator and the Coulomb potential. Due to much interest in the area, different approximate approaches were developed to tackle the solutions of other potentials whose analytic solutions

are difficult especially those potential models with centrifugal barriers. These different methods have different approaches to any given potential model but reproduce an equivalent result in terms of the wave functions and the energy eigenvalue numerically. One of such important potential is the inversely quadratic Yukawa potential model. The inversely quadratic Yukawa potential model has three parts. This comprises of the constant term, the exponential part, and the centrifugal barrier that serves as the denominator. The inversely quadratic Yukawa potential is a mathematical expression written in the form [1, 2]:

$$V(r) = \frac{V_0 e^{-2ar}}{r^2}. \quad (1)$$

\*Corresponding author: Tel.: +234-815-825-7734.

Email address: [adedewe.olorunfemi@Imu.edu.ng](mailto:adedewe.olorunfemi@Imu.edu.ng) (O. A. Adedewe)

The parameters in the potential are define as follows;  $V_0$  is the potential strength, that determines the range of the potential,  $r$  is the internuclear separation, and  $\alpha$  is the screening parameter. This potential finds applications in nuclear physics, atomic physics and condensed matter physics. The inversely quadratic Yukawa potential has not been adequately reported in the literature, this calls the attentions of the present study. Motivated by the applications of thermodynamic properties and Shannon entropy in science and engineering, the present study wants to examine the applicability of the inversely quadratic Yukawa potential for the thermodynamic properties and Shannon entropy. In this study, the energy eigenvalue equation and its corresponding wave function for the non-relativistic domain will be obtained using the popular parametric Nikiforov-Uvarov method (PNUM).

The energy equation will also be obtained using supersymmetric approach (SUSY). The details will not be given in the main text to avoid repetitions of terms but will be found in the appendix. The reason for the two methods is to compare the result to determine the accuracy of the energy equation. The obtained wave function and the energy level will be use to study Shannon entropy and thermodynamic properties respectively. Shannon entropy is a theoretic quantity that determines the uncertainty in a random variable as it measures the content of an information produced [3–10]. Shannon entropy finds applications in the information theory as well as computer science. In quantum mechanics, where potential models are involved the study of theoretic quantities, Shannon entropy is studied with a physical structure in the position space and momentum space, respectively, as

$$S(\rho) = -4\pi \int_0^{\infty} \rho(r) \log \rho(r) dr, \quad (2)$$

$$S(\gamma) = -4\pi \int_0^{\infty} \gamma(p) \log \gamma(p) dp. \quad (3)$$

The terms  $\rho(r)$  and  $\gamma(p)$  are the probability densities for position space and momentum space respectively. The probability densities are obtained from the wave functions. It has been shown that the accuracy of equation (2) and equation (3) for any potential can easily be verify by Bialynick-Birula, Mycielski inequality. The Bialynick-Birula, Mycielski inequality is of the form:

$$S(\rho) + S(\gamma) \geq 1 + \log \pi. \quad (4)$$

$S(\rho)$  is the Shannon entropy for the position space and  $S(\gamma)$  is the Shannon entropy in the momentum space. The physical meaning of equation (4) is that the sum of the Shannon entropy in the position space and the momentum space cannot be less than one plus the log of  $\pi$  for one dimensional system (the left-hand side cannot be less than the right-hand side). To ascertain the satisfactory condition of equation (4), one must compute numerical results for equation (2) and equation (3) as will be presented in this study.

## 2. Methodology

The energy equation and the wave function will explicitly be obtained by using parametric Nikiforov-Uvarov method. Without detail analysis, the energy equation of the same potential will be given by the method of supersymmetric approach. The parametric Nikiforov-Uvarov method is given by Tezcan and Sever[11, 12]. According to these authors, the standard equation is given as:

$$\psi''(s) + \frac{(x_1 - x_2 s)}{s(1 - x_3 s)} \psi'(s) + \frac{1}{s^2(1 - x_3 s)^2} [-p_0 s^2 + p_1 s - p_2] \psi(s) = 0. \quad (5)$$

Using equation (5), the authors gave the condition for energy equation and its corresponding wave function as:

$$x_2 n - (2n + 1)x_5 + [2x_8 + n(n - 1)]x_3 + x_7 + (2n + 1)\sqrt{x_9} + \sqrt{x_8} [2\sqrt{x_9} + x_3(2n + 1)] = 0, \quad (6)$$

$$\Psi(s) = N_{nl} s^{x_{12}} (1 - x_3 s)^{-x_{12} - \frac{x_{13}}{x_3}} P_n^{(x_{10}-1, \frac{x_{11}}{x_3} - x_{10}-1)}(1 - 2x_3 s) \quad (7)$$

The values of the parametric constants in equations (6) and (7) are obtained as follows:

$$\begin{aligned} x_1 &= x_2 = x_3 = 1, \quad x_4 = 0.5(1 - x_1), \quad x_5 = 0.5(x_2 - 2x_3), \\ x_6 &= x_5^2 + p_0, \quad x_7 = 2x_4 x_5 - p_1, \\ x_8 &= x_4^2 + p_2, \quad x_9 = x_3(x_7 + x_3 x_8) + x_6, \\ x_{10} &= x_1 + 2x_4 + 2\sqrt{x_8}, \quad x_{11} = x_2 - 2x_5 + 2(\sqrt{x_9} + x_3 \sqrt{x_8}), \\ x_{12} &= x_4 + \sqrt{x_8}, \quad x_{13} = x_5 - (\sqrt{x_9} + x_3 \sqrt{x_8}). \end{aligned} \quad (8)$$

## 3. Inversely quadratic Yukawa

To obtain the solutions of the radial Schrödinger equation with an inversely quadratic Yukawa potential, we write a Schrödinger equation with a radial potential  $V(r)$  as [13–15]:

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - E_{nl} + V(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell + 1)}{r^2} \right] R_{nl}(r) = 0, \quad (9)$$

where  $V(r)$  is the inversely quadratic Yukawa potential,  $E_{nl}$  is the energy in the non-relativistic domain,  $m$  is the particle mass,  $\hbar$  is the reduced Planck's constant,  $\ell$  is the angular momentum quantum number,  $n$  is the quantum number and  $R_{nl}(r)$  is the wave function. The centrifugal term in equation (1) and equation (9) can be approximated using the formula:

$$\frac{1}{r^2} = \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}. \quad (10)$$

The approximation scheme in equation (10) is valid for  $\alpha \ll 1$ . Substituting equation (1) and equation (10) into equation (9) and consider the transformation of the form  $s = e^{-2\alpha r}$ , we have a new equation of the form of equation (5):

$$\left[ \frac{d^2}{ds^2} + \frac{1-s}{s(1-s)} \frac{d}{ds} \right]$$

$$+ \frac{\left(\frac{m(E_{nl}+4V_0)}{2\alpha^2\hbar^2}\right)s^2 - \left(\frac{mE_{nl}}{\alpha^2\hbar^2} + \ell(\ell+1)\right)s + \frac{mE_{nl}}{2\alpha^2\hbar^2}}{s^2(1-s)^2} \Big] R_{n\ell}(s) = 0. \quad (11)$$

Comparing equation (11) with equation (5), the parametric constants in equation (8) become:

$$\begin{aligned} x_1 &= x_2 = x_3 = 1, \quad x_4 = 0, \quad x_5 = -\frac{1}{2}, \\ x_6 &= \frac{1}{4} - \frac{mE_{nl}}{2\alpha^2\hbar^2} - \frac{2mV_0}{\hbar^2} \\ x_7 &= \frac{mE_{nl}}{\alpha^2\hbar^2} + \ell(\ell+1), \quad x_8 = -\frac{mE_{nl}}{2\alpha^2\hbar^2}, \\ x_9 &= \ell(\ell+1) + \frac{1}{4} - \frac{2mV_0}{\hbar^2}, \quad x_{10} = 1 + 2\sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}} \\ x_{11} &= 2 + 2\sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}} + \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}}, \\ x_{12} &= \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}, \\ x_{13} &= -\frac{1}{2} - \frac{1}{2}\sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} - \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}. \end{aligned} \quad (12)$$

Plugging equation (12) into equation (6) and equation (7), respectively, we have the energy level and its corresponding wave function as:

$$E_{n,\ell}^{pm} = -\frac{2\alpha^2\hbar^2}{m} \left[ \frac{n(n+1) + \ell(\ell+1) + \frac{1}{2} + (n+\frac{1}{2})\sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}}}{1+2n + \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}}} \right]^2, \quad (13)$$

$$R_{n,\ell}(s) = NS \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}} (1-s)^{\frac{1}{2}+\frac{1}{2}} \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \times P_n \left[ \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}, \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \right] (1-2s). \quad (14)$$

To ascertain the accuracy of the energy equation in equation (13), the solution of the same potential is obtained using supersymmetry

$$E_{n,\ell}^{pm} = -\frac{\alpha^2\hbar^2}{2m} \left[ \frac{\frac{2mV_0}{\hbar^2} + \left(n + \frac{1}{2} + \frac{1}{2}\sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}}\right)^2}{n + \frac{1}{2} + \frac{1}{2}\sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}}} \right]^2. \quad (15)$$

The details of the calculation of equation (15) is presented in the appendix. To compute the Shannon entropy, the wave function in equation (14) is normalized using A MATHEMATICA software program. The components of the normalized wave function at different quantum states are given below:

$$R_{0,\ell}(s) = \sqrt{\frac{\alpha\Gamma[2(\lambda_1 + \lambda_2 + 1)]}{\Gamma(2\lambda_1)\Gamma(2\lambda_1)\Gamma(2\lambda_2 + 2)}} S \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}$$

$$(1-s)^{\frac{1}{2}+\frac{1}{2}} \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} P_n \left[ \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}, \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \right] (1-2s), \quad (16)$$

$$R_{1,\ell}(s) = \left[ \sqrt{\frac{2\alpha\lambda_1(2\lambda_1 + 2\lambda_2 + 3)\Gamma[2(\lambda_1 + \lambda_2 + 1)]}{(3 + 2\lambda_2)\Gamma(2\lambda_1 + 2)\Gamma(2\lambda_2 + 2)}} \right] \times S \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}} (1-s)^{\frac{1}{2}+\frac{1}{2}} \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \times P_n \left[ \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}, \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \right] (1-2s) \quad (17)$$

$$R_{2,\ell}(s) = \left[ \sqrt{\frac{4\alpha\lambda_1(2\lambda_1 + 2\lambda_2 + 5)\Gamma[2(\lambda_1 + \lambda_2 + 3)]}{(5 + 2\lambda_2)\Gamma(2\lambda_1 + 3)\Gamma(2\lambda_2 + 3)}} \right] \times S \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}} (1-s)^{\frac{1}{2}+\frac{1}{2}} \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \times P_n \left[ \sqrt{-\frac{mE_{nl}}{2\alpha^2\hbar^2}}, \sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \right] (1-2s). \quad (18)$$

### 3.1. Thermodynamic properties

This section deals with the computation of some thermodynamic properties such as vibrational enthalpy, Gibbs free energy and entropy. The computation of these properties strongly depends on the vibrational partition function. To calculate the vibrational partition function, we re-write the energy equation in equation (15) as:

$$E_{n\ell}(s) = -\frac{\alpha^2\hbar^2}{2m} \left( \frac{\theta_0}{n} - (n + \delta) \right)^2, \quad (19)$$

where we have defined the following for simplicity

$$\theta_0 = \frac{2mV_0}{\hbar^2}, \quad \delta = \left( \frac{1}{2} + \frac{1}{2}\sqrt{(1+2\ell)^2 - \frac{8mV_0}{\hbar^2}} \right)^2. \quad (20)$$

The the vibrational partition function for the energy level  $E_{n\ell}$  with physical potential is written as [16–25]:

$$Z = \sum_{n=0}^{n_{max}} e^{-\beta E_{n\ell}}, \quad (21)$$

where  $\beta = \frac{1}{K_B T}$ ,  $K_B$  is the Boltzmann constant and  $T$  is the absolute temperature. The term  $n_{max}$  is the maximum quantum state obtained from the solution of  $\frac{dE_{n\ell}}{dn} = 0$ . Using Poisson summation, equation (21) can be written in the form:

$$Z = \sum_{n=0}^{n_{max}} e^{-\beta E_{n\ell}} = \sum_{n=0}^{n_{max}} f(n) = \frac{1}{2} [f(0) - f(n_{max} + 1)] + \int_0^{n_{max}+1} f(y) dy, \quad (22)$$

where  $f(n) = e^{\theta \left( \frac{\theta_0}{n+\delta} - n - \delta \right)^2}$ ,  $\theta^2 = \frac{\beta\alpha^2\hbar^2}{2m}$  and  $n_{max} = \sqrt{\theta_0} + \delta$ . Plugging equation (19) into equation (22), we have

$$Z = \frac{1}{2} \left[ e^{\alpha\hbar\theta\theta_1^2} - e^{\alpha\hbar\theta\theta_2^2} + \frac{\sqrt{\pi} (erfi(\theta\theta_1) - erfi(\theta\theta_2))}{\theta} \right], \quad (23)$$

Table 1: Energy of the inversely quadratic Yukawa potential from PNUM method and SUSY method for various state as a function of the screening parameter with ( $m = \hbar = 1$ ).

State	$\alpha$	$V_0 = 1.5, E_{n,\ell}^{pm}$	$V_0 = 1.5, E_{n,\ell}^{sm}$	$V_0 = 2.5, E_{n,\ell}^{pm}$	$V_0 = 2.5, E_{n,\ell}^{sm}$
2p	0.05	-0.0012500	-0.0012500	-0.0006944	-0.0006944
	0.15	-0.0112500	-0.0112500	-0.0062500	-0.0062500
	0.25	-0.0312500	-0.0312500	-0.0173611	-0.0173611
3p	0.05	-0.0112500	-0.0012500	-0.0112500	-0.0112500
	0.15	-0.1012500	-0.1012500	-0.1012500	-0.1012500
	0.25	-0.2812500	-0.2812500	-0.2812500	-0.2812500
3d	0.05	-0.0162500	-0.0162500	-0.0277090	-0.0182253
	0.15	-0.1462500	-0.1462500	-0.2493808	-0.1640278
	0.25	-0.4062500	-0.4062500	-0.6927245	-0.4556327
4p	0.05	-0.0156378	-0.0156378	-0.0182253	-0.0256269
	0.15	-0.1407398	-0.1407398	-0.1640278	-0.2306425
	0.25	-0.3909439	-0.3909439	-0.4556327	-0.6406735
4d	0.05	-0.0221667	-0.0221667	-0.0256269	-0.0256269
	0.15	-0.1995006	-0.1995006	-0.2306425	-0.2306425
	0.25	-0.5541683	-0.5541683	-0.6406735	-0.6406735
4f	0.05	-0.0240738	-0.0240738	-0.0283067	-0.0283067
	0.15	-0.2166638	-0.2166638	-0.2547601	-0.2547601
	0.25	-0.6018439	-0.6018439	-0.7076671	-0.7076671

Table 2: Computation for the uncertainty relation  $S(\rho) + S(\gamma) \geq 1 + \log \pi$  as a function of the potential strength at the ground state with ( $m = \hbar = 1, \alpha = 0.2$ , and  $\ell = 0$ ).

$V_0$	$S(\rho)$	$S(\gamma)$	$S(\rho) + S(\gamma)$
0.01	59.7713	-22.9178	36.8536
0.02	59.2309	-22.6164	36.6145
0.03	58.6597	-22.3001	36.3596
0.04	58.0525	-21.9664	36.0861
0.05	57.4025	-21.6120	35.7905
0.06	56.7009	-21.2327	35.4682
0.07	55.9349	-20.8224	35.1125
0.08	55.0856	-20.3720	34.7136
0.09	54.1228	-19.8672	34.2557
0.10	52.9923	-19.2820	33.7103

Table 3: Computation for the uncertainty relation  $S(\rho) + S(\gamma) \geq 1 + \log \pi$  as a function of the screening parameter at the ground state with ( $m = \hbar = 1, V_0 = -0.2$ , and  $\ell = 0$ ).

$\alpha$	$S(\rho)$	$S(\gamma)$	$S(\rho) + S(\gamma)$
0.01	47169.20	-71.5345	47097.6
0.02	10627.40	-61.3486	10566.1
0.03	4420.470	-55.3902	4365.07
0.04	2365.650	-51.1627	2314.48
0.05	1454.010	-47.8835	1406.13
0.06	975.688	-45.2043	930.484
0.07	695.685	-42.9390	652.746
0.08	518.609	-40.9768	477.632
0.09	399.990	-39.2459	360.744
0.10	316.910	-37.6976	279.212

Table 4: Computation for the uncertainty relation  $S(\rho) + S(\gamma) \geq 1 + \log \pi$  as a function of the screening parameter at the first excited state with ( $m = \hbar = 1, V_0 = -0.2$ , and  $\ell = 0$ ).

$\alpha$	$S(\rho)$	$S(\gamma)$	$S(\rho) + S(\gamma)$
0.01	27482.8	-43.1157	27439.7
0.02	6085.37	-34.4936	6050.88
0.03	2500.44	-29.4500	2470.99
0.04	1325.01	-25.8715	1299.14
0.05	807.556	-23.0959	784.46
0.06	537.851	-20.8280	517.023
0.07	380.898	-18.9105	361.988
0.08	282.170	-17.2495	264.92
0.09	216.359	-15.7844	200.575
0.10	170.476	-14.4738	156.002

where we have made the following transformation to obtained equation (23) above

$$\theta_1 = \frac{\theta_0 - \delta^2}{\delta}, \quad \theta_2 = \frac{\theta_0 - (n_{max} + 1 + \delta)^2}{(n_{max} + 1 + \delta)}. \tag{24}$$

### 3.2. Vibrational enthalpy ( $H_v$ )

The vibrational enthalpy is given by:

$$H_v = RT^2 \left( \frac{\partial}{\partial T} \ln Z \right) = \frac{\Theta_0 RT^2 + \Theta_1 RT^2 + \Theta_2 RT^2}{\frac{e^{\frac{\alpha \hbar \omega_1^2}{2}} - e^{\frac{\alpha \hbar \omega_2^2}{2}}}{2} + \frac{\sqrt{\pi} (erfi(\theta_1) - erfi(\theta_2))}{2\theta}}. \tag{25}$$

### 3.3. Vibrational Gibbs free energy ( $G_v$ )

The vibrational Gibbs free energy is given by

$$G_v = -RT \ln Z =$$

Table 5: Computation for the uncertainty relation  $S(\rho) + S(\gamma) \geq 1 + \log \pi$  as a function of the screening parameter at the second excited state with ( $m = \hbar = 1$ ,  $V_0 = -0.2$ , and  $\ell = 0$ ).

$\alpha$	$S(\rho)$	$S(\gamma)$	$S(\rho) + S(\gamma)$
0.01	23705.4	-42.5877	2366.90
0.02	5204.31	-33.3635	5170.95
0.03	2125.3	-27.9677	2097.34
0.04	1120.56	-24.1393	1096.42
0.05	679.969	-21.1698	658.799
0.06	451.098	-18.7435	432.354
0.07	318.310	-16.6921	301.618
0.08	235.013	-14.9151	220.097
0.09	179.630	-13.3477	166.282
0.10	141.110	-11.9456	129.164

Table 6: Computation of vibrational enthalpy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), Gibbs free energy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), and entropy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), with ( $m = \ell = \hbar = 1$ ,  $V_0 = 2$ ,  $R = 8.31446\text{JMol}^{-1}\text{K}^{-1}$ , and  $\alpha = 0.25$ ) as a function of temperature

$T$	H	$-G$	$S$
100	423.4262683	2571.207395	29.98630609
200	839.7276665	5743.153705	32.91440684
300	1255.704638	9111.968879	34.55891173
400	1671.563775	12614.53764	35.75526869
500	2087.371906	16254.18773	36.68311926
600	2503.153570	19937.54615	37.44117568
700	2918.913234	23738.53963	38.08207550
800	3334.664349	27543.11291	38.67937166
900	3750.404032	31463.81012	39.12690463
1000	4166.136431	35400.91769	39.56492493

$$-RT \ln \left[ \frac{e^{\alpha \hbar \theta_1^2}}{2} - \frac{e^{\alpha \hbar \theta_2^2}}{2} + \frac{\sqrt{\pi} (erfi(\theta \theta_1) - erfi(\theta \theta_2))}{2\theta} \right] \quad (26)$$

### 3.4. Vibrational entropy ( $S_v$ )

The vibrational entropy is given by

$$S_v = R \ln Z + RT \left( \frac{\partial}{\partial T} \ln Z \right) \\ = R \ln \left[ \frac{e^{\alpha \hbar \theta_1^2}}{2} - \frac{e^{\alpha \hbar \theta_2^2}}{2} + \frac{\sqrt{\pi} (erfi(\theta \theta_1) - erfi(\theta \theta_2))}{2\theta} \right] + \frac{H_v}{T} \quad (27)$$

## 4. Discussion

The comparative of the energy eigenvalue of the inversely quadratic Yukawa potential from PNUM and SUSY as a function of the screening parameter for various states with two values of the potential strength are presented in Table 1. The essence of this table is to test the accuracy of the energy equation. The energy from PNUM is given in equation (13) while the energy from SUSY is given in equation (15). The results

Table 7: Computation of vibrational enthalpy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), Gibbs free energy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), and entropy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), with ( $m = \ell = \hbar = 1$ ,  $V_0 = 2$ ,  $R = 8.31446\text{JMol}^{-1}\text{K}^{-1}$ , and  $T = 500\text{K}$ ), as a function of the screening parameter.

$\alpha$	H	$-G$	$S$
0.5	2110.267247	13347.70080	30.91593619
1.5	2212.249858	8603.087528	21.63067478
2.5	1984.436099	6382.143396	16.78039394
3.5	1344.257611	5263.754858	13.21602496
4.5	885.2891146	4690.735238	11.21699192
5.5	1024.410818	4355.348694	10.75951902
6.5	1741.590440	3894.863342	11.27290756
7.5	3235.440468	3214.514258	12.89990946
8.5	5790.081022	2122.365386	15.61919559
9.5	10717.00589	429.2341956	22.15933013

Table 8: Computation of vibrational enthalpy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), Gibbs free energy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), and entropy ( $\text{JMol}^{-1}\text{K}^{-1}$ ), with ( $m = \ell = \hbar = 1$ ,  $\alpha = 0.25$ ,  $R = 8.31446\text{JMol}^{-1}\text{K}^{-1}$ , and  $T = 500\text{K}$ ), as a function of the potential strength.

$V_0$	H	$-G$	$S$
5	-1520.089822	7118.650061	17.21039174
10	-722.1248949	6142.296830	13.728840218
15	120.5879918	6217.726156	12.13186401
20	1023.718885	6756.765215	11.46609509
25	2005.842767	7578.130088	11.14457213
30	3026.796524	8633.357447	11.21312509
35	4073.416666	9781.742465	11.42001802
40	5273.526590	11091.84695	11.74306044
45	6539.050687	12571.51523	12.06494150
50	7792.441709	14056.38031	12.54057090

of the two methods are exactly the same for all states. This confirmed that the two energy equations are correct.

The eigenvalue reduces in magnitude as both  $n$  and  $\alpha$  as well as  $\ell$  respectively increases. The energies with  $V_0 = 1.5$  are higher than the energies obtained with  $V_0 = 2.5$  for 2p state. For the 3p state, the energies obtained with the two values of  $V_0$  are the same. For 3d, 4p, 4d and 4f states, the energies obtained with  $V_0 = 2.5$  are higher than the energies obtained with  $V_0 = 1.5$ . The results of Shannon entropy for position space, momentum space and their sum as a function of the potential strength  $V_0$  at the ground state are presented in Table 2. At different values of  $V_0$ , the position space and momentum space Shannon entropy vary inversely with each other, showing associability of the diffused density distribution of the momentum space with the localized density distribution of the position space. The results also revealed that the momentum space Shannon entropy are completely bounded with squeezing effect at all values of  $V_0$ .

The results satisfied the Bialynick-Birula, Mycielski (BBM) inequality given in equation (4) with a lower bound of 33.7103. However, for excited states, the uncertainty principle and BBM inequality are not satisfied. In Table 3, Table 4 and Table 5, re-



spectively, the numerical values for Shannon entropy as a function of the screening  $\alpha$  parameter for  $n = 0$ ,  $n = 1$  and  $n = 2$  are presented. The behaviours observed in Table 2 are also observed in Tables 3, 4 and 5. The variation of the Shannon entropy for both the position space and momentum space against  $\alpha$  for all the ground state and the excited states obeyed the BBM inequality with the lower bound above  $1 + \log\pi$ .

However, it is noticed that the higher the quantum state, the lower the Shannon entropy in position space but the higher the Shannon entropy in momentum space. The Shannon entropy for the momentum space is purely negative with both the potential strength and the screening parameter. The numerical values for the vibrational enthalpy, Gibbs free energy and entropy are obtained using equations (25), (26) and (27), respectively. The numerical values as a function of  $T$ ,  $\alpha$  and  $V_0$  are presented in Tables 6, 7 and 8, respectively. In Table 6, the enthalpy and entropy respectively increase positively as the temperature rises but the Gibbs free energy increases negatively. This is the exact trends obtained for molecular potential when the predicted results are compared with the experimental values [26, 27]. However, in Tables 7 and 8, where the thermodynamic properties are examined as a function of the screening parameter and the potential strength, the trends differ.

The variation of the enthalpy and entropy as a function of  $\alpha$ , is not in one direction but that of the Gibbs free energy increases with increase in  $\alpha$ . A critical observation shows that the vibrational Gibbs free energy tends towards positive as  $\alpha$  increases significantly. In Table 8 there is no constant variation in all the thermodynamic properties. However, the Gibbs free energy is positive for all values of  $V_0$ .

## 5. Conclusion

The solutions for inversely quadratic Yukawa potential are obtained via two traditional approaches. The two approaches reproduced agreeable numerical values for the energy of the interacting potential. The energy of the potential is fully bounded and reduces with increase in most of the parameters. The results of Shannon entropy for both the configuration space and momentum space as a function of the screening parameter satisfied the Bialynick-Birula, Mycielski inequality for all quantum states, however, the results of Shannon entropy for both the configuration space and momentum space as a function of the potential strength only satisfied the theBialynick-Birula, Mycielski inequality at the ground state. This shows that as the quantum number increases, the sum of the Shannon entropies reduces beyond  $1 + \log\pi$ . The thermodynamic properties studied as a function of temperature followed the trends of the molecular potential studied and compared with experimental data even though the potential here is not a molecular potential [26, 27].

## References

[1] M. Hamzavi, S. M. Ikhdair & B. I. Ita, "Approximate spin and pseudospin solutions to the Dirac equation for the inversely quadratic Yukawa potential and tensor interaction", *Physica Scripta* **85** (2012) 045009. <https://doi.org/10.1088/0031-8949/85/04/045009>.

[2] C. A. Onate, "Relativistic and Non-relativistic Solutions of the Inversely Quadratic Yukawa Potential", *African Review of Physics* **8** (2013) 325.

[3] A. Orłowski, "Information entropy and squeezing of quantum fluctuations", *Physical Review A* **56** (1997) 2545. <https://doi.org/10.1103/PhysRevA.56.2545>.

[4] E. Omugbe, O. E. Osafire, I. J. Njoku, A. Jahanshir, C. O. Edet, I. B. Okon, E. S. Eyube, C. A. Onate, R. Horchani, E. S. William & A. N. Ikot, "Information-theoretic measures and thermodynamic properties under magnetic and Aharonov-Bohm flux fields", *European Physical Journal D* **77** (2023) 143. <https://doi.org/10.1140/epjd/s10053-023-00718-1>.

[5] M. C. Onyeaju, E. Omugbe, C. A. Onate, I. B. Okon, E. S. Eyube, U. S. Okorie, A. N. Ikot, D. A. Ogwu & O. P. Osohor, "Information Theory and thermodynamic properties of diatomic molecules using Molecular potential", *Journal of Molecular Modeling* **29** (2023) 311. <https://doi.org/10.1007/s00894-023-05708-z>

[6] C. A. Onate, I. B. Okon, U. E. Vincent, E. Omugbe, E. S. Eyube, M. C. Onyeaju & G. O. Jude, "Theoretic measure and thermal properties of a standard Morse potential model", *Journal of Molecular Modeling* **29** (2023) 34. <https://doi.org/10.1007/s00894-022-05441-z>.

[7] J. S. Dehesa, I. V. Toranzo & D. Puertas-Centeno, "Entropic measures of Rydberg-like harmonic states", *International Journal of Quantum Chemistry* **117** (2017) 48. <https://doi.org/10.1002/qua.25315>.

[8] W. A. Yahya, K. J. Oyewumi & K. D. Sen, "Quantum information entropies for the state Pöschl Teller-type potential", *Journal of Mathematical Chemistry* **54** (2016) 1810. <https://doi.org/10.1007/s10910-016-0650-7>.

[9] S. A. Najafzade, H. Hassanabadi & S. Zarrinkamar, "Nonrelativistic Shannon information entropy for Kratzer potential", *Chinese Physics B* **25** (2016) 040301. <https://doi.org/10.1088/1674-1056/25/4/040301>.

[10] J. S. Dehesa, W. W. Assche & R. J. Yanez, "Information entropy of classical orthogonal polynomials and their application to the harmonic oscillator and Coulomb potentials", *Methods and Applications of Analysis* **4** (1997) 91. <https://dx.doi.org/10.4310/MAA.1997.v4.n1.a7>.

[11] C. Tezcan & R. Sever, "A General Approach for the exact Solution of the Schrödinger equation", *International Journal of Theoretical Physics* **48**(2009) 337. <https://doi.org/10.1007/s10773-008-9806-y>.

[12] C. A. Onate, M. O. Oluwayemi & I. B. Okon, "Dirac Equation for Energy-Dependent Potential with Energy-dependent Tensor Interaction", *Journal of the Nigerian Society of Physical Sciences* **5** (2023) 917. <https://doi.org/10.46481/jnsp.2023.917>.

[13] O. Bayrak, I. Boztosun & H. Ciftci, "Exact Analytical Solutions to the Kratzer Potential by the asymptotic iteration method", *International Journal of Quantum Chemistry* **107** (2007) 540. <https://doi.org/10.1002/qua.21141>.

[14] X. Y. Gu, S. H. Dong & Z. Q. Ma, "Energy spectra for modified Rosen-Morse potential solved by the exact quantization rule", *Journal of Physics A Mathematics and Theoretical* (2009) 035303. <https://doi.org/10.1088/1751-8113/42/3/035303>.

[15] W. C. Qiang & S. H. Dong, "Proper quantization rule", *EPL* **89** (2010) 10003. <https://doi.org/10.1209/0295-5075/89/10003>.

[16] S. H. Dong, R. Lemus & A. Frank, "Ladder operators for the Morse potential", *International Journal of Quantum Chemistry* **86** (2002) 433. <https://doi.org/10.1002/qua.10038>.

[17] S. H. Dong, "The SU (2) realization for the Morse potential and its coherent states", *Canadian Journal of Physics* **80** (2002) 129. <https://doi.org/10.1139/p01-130>.

[18] G. H. Liu, Q. C. Ding, C. W. Wang & C. S. Jia, "Unified explicit formulations of thermodynamic properties for the gas  $NO_2$ , and gaseous  $BF_2$  and  $AlCl_2$  radicals", *Chem. Phys. Lett.* **830** (2023) 140788. <https://doi.org/10.1016/j.cplett.2023.140788>.

[19] G. H. Liu, Q. C. Ding, C. W. Wang & C. S. Jia, "Unified non-fitting explicit formulation of thermodynamic properties for five compounds", *Journal of Molecular Structure* **1294** (2023) 136543. <https://doi.org/10.1016/j.molstruc.2023.136543>.

[20] Q. C. Ding, C. W. Wang, X. L. Peng, Y. Y. Lu, G. H. Liu, G. Li, L.S. Wei, J.Q. Chen. H. Yuan & C. S. Jia, "Unified analytical formulation regarding thermodynamic properties subject to gaseous metal hydroxides", *Journal of Molecular Structure* **1298** (2024) 137075. <https://doi.org/10.1016/j.molstruc.2023.137075>.

- [21] C. W. Wang, X. L. Peng, J. Y. Liu, R. Jiang, X. P. Li, Y. S. Liu, S. Y. Liu, L. S. Wei, L. H. Zhang & C. S. Jia, "A novel formulation representation of the equilibrium constant for water gas shift reaction ", *International Journal of Hydrogen Energy* **47** (2022) 27821. <https://doi.org/10.1016/j.ijhydene.2022.06.105>.
- [22] C. W. Wang, J. Li, L. H. Zhang, Q. C. Ding, G.H Liu, G. Li, R. Jiang, X. L. Peng, L. S. Wei, H. M. Tang, J. Y. Liu & C. S. Jia, "Non-fitting functional representation for the equilibrium constant subject to reaction between  $H_2S$  and  $CO_2$ ", *Fuel* **362** (2024) 130916. <https://doi.org/10.1016/j.fuel.2024.130918>.
- [23] S. H. Dong & M. Cruz. Irisson, "Energy spectrum for a modified Rosen-Morse potential solved by proper quantization rule and its thermodynamic properties ", *Journal of Mathematical Chemistry* **50** (2012) 881. <https://doi.org/10.1007/s10910-011-9931-3>.
- [24] S. H. Dong, M. Lozada-Cassou, J. Yu, F. Jimenze-Angeles & A. L. Rivera, "Hidden symmetries and thermodynamic properties for a harmonic oscillator plus an inverse square potential", *International Journal of Quantum Chemistry* **107** (2007) 366. <https://doi.org/10.1002/qua.21103>.
- [25] M. Buchowiecki, "Ro-vibrational coupling in high temperature thermochemistry of the BBr Molecule", *Chem. Phys. Lett.* **692** (2018) 236 <https://doi.org/10.1016/j.cplett.2017.12.051>.
- [26] C. A. Onate, I. B. Okon, E. Omugbe, E. S. Eyube, B. A. AL-Asbahi, Y. A. Kumar, K. O. Emeje, E. Aghemenloh, A. R. Obasuyi, V. O. Obaje & T. O. Etchie. "Theoretical prediction of molar entropy of modified shifted Morse potential for gaseous molecules", *Chem. Phys.* **582** (2024) 112294. <https://doi.org/10.1016/j.chemphys.2024.112294>.
- [27] Q. C. Ding, C. W. Wang, X. L. Peng, Y. Y. Lu, G. H. Liu, G. Li, L. S. Wei, J.Q. Chen, H. Yuan & C. S. Jia, "Unified analytical formulation regarding thermodynamic properties subject to gaseous metal hydroxides", *J. Mol. Struct.* **1298** (2024) 137075. <https://doi.org/10.1016/j.molstruc.2023.137075>.

## Appendix A

Solutions of the Schrödinger equation with inversely quadratic Yukawa potential using supersymmetric quantum mechanics approach. The radial Schrödinger equation is given by:

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - E_{n\ell} + V(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right] R_{n\ell}(r) = 0. \quad \text{A1}$$

The interacting potential and the approximation scheme, respectively, are given by:

$$V(r) = \frac{V_0 e^{-2\alpha r}}{r}, \quad \text{A2}$$

$$\frac{1}{r^2} = \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}. \quad \text{A3}$$

Substituting equation (A2) and equation (A3) into equation (A1), gives a new equation of the form

$$\frac{d^2 R_{n,\ell}(r)}{dr^2} = \left[ \frac{(4\ell(\ell+1)\alpha^2 - \frac{8mV_0\alpha^2}{\hbar^2}) e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} + \frac{8mV_0\alpha^2 e^{-2\alpha r}}{\hbar^2 (1 - e^{-2\alpha r})} - \frac{2mE_{n,\ell}}{\hbar^2} \right] R_{n,\ell}(r) \quad \text{A4}$$

To proceed from equation (A4), we write the ground state wave function for the system as

$$R_{0,\ell}(r) = e^{-\int W(r) dr}, \quad \text{A5}$$

where  $W(r)$  is the superpotential function. Substituting equation (A5) into equation (A4) after some mathematical simplifications gives

$$W^2(r) - \frac{dW(r)}{dr} = \frac{(4\ell(\ell+1)\alpha^2 - \frac{8mV_0\alpha^2}{\hbar^2}) e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} + \frac{8mV_0\alpha^2 - 2mE_{n,\ell}(1 - e^{-2\alpha r})}{\hbar^2 (1 - e^{-2\alpha r})}. \quad \text{A6}$$

Using the method and formalism of supersymmetric approach, the solution to equation (A6) is the superpotential function. Considering the interacting potential and Riccati equation (A6), we proposed a superpotential function as:

$$\lambda_0 + \frac{\lambda_1 e^{-2\alpha r}}{1 - e^{-2\alpha r}}, \quad \text{A7}$$

where  $\lambda_0$  and  $\lambda_1$  are superpotential constants. Substituting equation (A7) into equation (A6), after a series of mathematical manipulations and simplifications, the two superpotential constants in equation (15) are obtained as follow:

$$\lambda_0^2 = \frac{-2mE_{n,\ell}}{\hbar^2}, \quad \text{A8}$$

$$\lambda_1 = \alpha \left( 1 \pm \sqrt{(2\ell+1)^2 - \frac{8mV_0}{\hbar^2}} \right), \quad \text{A9}$$

$$\lambda_0 = \frac{\frac{4\mu V_0 \alpha^2}{\hbar^2} + \lambda_1^2}{\lambda_1}. \quad \text{A10}$$

Using equation (A7), the supersymmetric family potentials can conveniently be constructed as:

$$V_+(r) = W^2(r) + \frac{dW(r)}{dr} = \lambda_0^2 + \frac{\lambda_1(2\lambda_0 - \lambda_1)e^{-2\alpha r}}{1 - e^{-\alpha r}} + \frac{\lambda_1(\lambda_1 - 2\alpha)e^{-\alpha r}}{(1 - e^{-\alpha r})^2}, \quad \text{A11}$$



$$V_-(r) = W^2(r) - \frac{dW(r)}{dr} = \lambda_0^2 + \frac{\lambda_1(2\lambda_0 - \lambda_1)e^{-2\alpha r}}{1 - e^{-\alpha r}} + \frac{\lambda_1(\lambda_1 + 2\alpha)e^{-\alpha r}}{(1 - e^{-\alpha r})^2}. \tag{A12}$$

The family potentials satisfied the invariant condition via mapping of the form  $\lambda_1 \rightarrow \lambda_1 + 2\alpha$ . Where  $\lambda_1 = a_0$ . This implies that  $a_1 = f(a_0) = a_0 + 2\alpha$ , where  $a_1$  is new set of parameters uniquely determined from  $a_0$  an old set of parameters. Since  $a_1 = a_0 + 2\alpha$ , it follows that  $a_2 = a_0 + 4\alpha$ ,  $a_3 = a_0 + 6\alpha$ ,  $a_4 = a_0 + 8\alpha$ , and subsequently,  $a_n = a_0 + 2\alpha n$ . However, the family potentials are related by the formula:

$$V_+(a_0, r) = V_-(a_0, r) + R(a_1), \tag{A13}$$

which is a residual term that is completely independent of the variable  $r$ . Equation (A13) can be written in a recurrence relation of the form:

$$R(a_1) = \left( \frac{\frac{4mV_0\alpha^2}{\hbar^2} + a_0^2}{a_0} \right)^2 - \left( \frac{\frac{4mV_0\alpha^2}{\hbar^2} + a_1^2}{a_1} \right)^2 \tag{A14}$$

$$R(a_2) = \left( \frac{\frac{4mV_0\alpha^2}{\hbar^2} + a_1^2}{a_1} \right)^2 - \left( \frac{\frac{4mV_0\alpha^2}{\hbar^2} + a_2^2}{a_2} \right)^2, \tag{A15}$$

$$R(a_n) = \left( \frac{\frac{4mV_0\alpha^2}{\hbar^2} + a_{n-1}^2}{a_{n-1}} \right)^2 - \left( \frac{\frac{4mV_0\alpha^2}{\hbar^2} + a_n^2}{a_n} \right)^2, \tag{A16}$$

The complete energy level for inversely quadratic Yukawa potential can be obtain following:

$$E_{n,\ell} = \sum_{k=1}^n = R(a_1) + R(a_2) + R(a_3) + \dots + R(a_n), \tag{A17}$$

which gives the real energy as:

$$E_{n,\ell}^{pm} = -\frac{\alpha^2 \hbar^2}{2m} \left[ \frac{\frac{2mV_0}{\hbar^2} + \left( n + \frac{1}{2} + \frac{1}{2} \sqrt{(1 + 2\ell)^2 - \frac{8mV_0}{\hbar^2}} \right)^2}{n + \frac{1}{2} + \frac{1}{2} \sqrt{(1 + 2\ell)^2 - \frac{8mV_0}{\hbar^2}}} \right]^2. \tag{A18}$$