SHANNON ENTROPY AND INFORMATION ENERGY FOR MODIFIED MANNING-ROSEN POTENTIAL

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ABSTRACT

The bound state solutions of the l-wave Schrodinger equation for modified Manning-Rosen potential are obtained using a proper approximation scheme to the centrifugal term. This potential model is of great significant in the description of vibrational energy levels of diatomic molecules. The energy spectrum formula and normalized wave functions expressed in terms of the Jacobi polynomial are obtained by application of parametric Nikiforov - Uvarov (NU) method. To show further application of our work, we have computed the Shannon entropy and information energy of the modified Manning-Rosen potential. We have also applied our results to the computation of the energy spectra of three diatomic molecules HCl, LiH and CO which have significant applications in atomic and molecular physics, chemical physics, quantum chemistry and other related areas.

INTRODUCTION

One of the main task of quantum mechanics is to find exact solutions of the wave equations for certain type of potentials of physical interest since they contain all the necessary information regarding the quantum system under consideration (Schiff, 1968; Dong, 2003; Ikhdair and Sever, 2008a; Berkdemir, 2007; Qiang and Dong, 2009; Wei *et al.,* 2009). In most of the solutions of the Schrodinger equation in the presence of the most typical potential model, the use of approximation scheme is inevitable. Among these potentials is the Morse potential (Morse, 1929).

The exact solutions of these wave equations are only possible in a few simple cases such as the Coulomb, Harmonic Oscillator, Pseudo harmonic and Mie-type potentials (Wei *et al*., 2007; Dong *et al*., 2003; Ikhdair and Sever, 2007; Ikhdair and Sever, 2008b). For an arbitrary l-state, most quantum systems could be only treated by approximation method. In recent years, many authors have studied the non-relativistic and relativistic wave equations with certain potentials for the s- and l - waves and the exact and approximate solutions obtained analytically (Ikot *et al.*, 2011; Ikot *et al.*, 2013; Awoga *et al*., 2012; Antia *et al*., 2013; Oyewumi *et al*., 2008; Hamzavi and Rajabi, 2011).

For instance, Ikhdair (2011), obtained bound state solutions of the Schrodinger equations with Manning-Rose potential and generated eigenvalues for twelve diatomic molecules. Falaye *et.al*., (2013) investigated bound state solutions of the Schrodinger equations in the presence of Manning-Rosen potential with three different approximation schemes to the centrifugal term.
Chen *et al.*, (2013) studied position-momentum uncertainty relations for a Poschl-Teller potential and it's squeezed phenomena. Ikot and Akpan (2012), obtained bound state solution of the Schrodinger equation for a more general Woods-Saxon potential with the arbitrary l-state.

The Nikiforov-Uvarov (NU) method, which is one of the methods of solving second order differential equations is very useful in calculating the exact energy levels of all bound states for some solvable quantum system. Motivated by the considerable interest in exponential type potentials, we attempt to study the quantum properties of exponential-type potential proposed by Manning and Rosen (Mehnet and Harun, 2004).

$$V(r)=V_0\left(\frac{\alpha(\alpha-1)e^{-2r/b}}{\left(1-e^{-r/b}\right)^2}-\frac{\beta e^{-r/b}}{\left(1-e^{r/b}\right)}\right), V_0=\frac{\hbar^2}{2\mu b^2} \quad (1)$$

while β and α are two dimensionless parameter, but the screening parameter b has dimension of length and correspond to the potential range. It is also used in several branches of physics for their bound states and scattering properties.

In our analysis we find that the potential remains invariant by mapping $\propto\to 1-\propto$, and the second derivative that determines the force constants at $r=r_0$ is given by

$$\left.\frac{d^2V}{dr^2}\right|_{r=r_0}=\frac{\beta^2[\beta+2\alpha(\alpha-1)]^2}{8b^4\alpha^3(\alpha-1)^3} \quad (2)$$

The purpose of this paper is to investigate the l-state solutions of Schrödinger equation with modified Manning-Rosen potential within the NU framework to generate energy spectrum and apply the solutions to obtain Shannon entropy and information energy for the system.

COMPUTATIONAL DETAILS

Parametric Nikiforov – Uvarov Method

The NU method is based on solving the hyper-geometric type second order differential equation (Nikiforov and Uvarov, 1988). Employing an appropriate coordinate transformation $z=z(r)$, we may rewrite Schrodinger equation using the parametric generalization of the NU method as (Tezcan and Sever, 2009)

$$\psi_n''(z)+\frac{(c_1-c_2z)}{z(1-c_3z)}\psi_n'(z)+\frac{1}{z^2(1-c_3z)^2}\left[-\xi_1z^2+\xi_2z-\xi_3\right]\psi(z)=0 \quad (3)$$

According to the NU method, the energy eigenvalues equation and eigen functions respectively satisfy the following set of equations

$$c_2n-(2n+1)c_5+(2n+1)\left(\sqrt{c_9}+c_3\sqrt{c_8}\right)+n(n-1)c_3+c_7+2c_3c_8+2\sqrt{c_8c_9}=0 \quad (4)$$

$$\psi_n(z)=N_{nl}\,Z^{c_{12}}(1-c_3z)^{-c_{12}-\frac{c_{13}}{c_3}}P_n^{\left(c_{10}-1,\frac{c_{11}}{c_3}-c_{10}-1\right)}(1-2c_3z) \quad (5)$$

where

$$c_4=\frac{1}{2}(1-c_1),\ c_5=\frac{1}{2}(c_2-2c_3),\ c_6=c_5^2+\xi_1,\ c_7=2c_4c_5-\xi_2,$$
$$c_8=c_4^2+\xi_3,\ c_9=c_3c_7+c_3^2c_8+c_6, c_{10}=c_1+2c_4+2\sqrt{c_8}, \quad (6)$$
$$c_{11}=c_2-2c_5+2\left(\sqrt{c_9}+c_3\sqrt{c_8}\right), c_{12}=c_4+\sqrt{c_8},\ c_{13}=c_5-\left(\sqrt{c_9}+c_3\sqrt{c_8}\right)$$

and $P_n^{(\alpha,\beta)}$ is the orthogonal Jacobi Polynomial.

Eigen Solutions of modified Manning-Rosen potential

In other to obtain the solution of these potential, we write the three-dimensional Schrödinger equation

$$\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)\right]\psi_{n,l,m}(r)=[E-V(r)]\psi_{n,l,m}(r) \quad (7)$$

Setting the wave function as

$$\psi_{n,l,m}(r)=\frac{R_{n,l}(r)Y_{l,m}(\theta,\phi)}{r} \quad (8)$$

We obtain the radial part of the Schrödinger equation by separation of variables as

$$\frac{d^2R_{n,l}(r)}{dr^2}+\left[\frac{2\mu}{\hbar^2}\left(E_{n,l}-V(r)\right)-\frac{l(l+1)}{r^2}\right]R_{n,l}(r)=0 \tag{9}$$

Inserting the potential in Eq. (1) into Eq. (9), we have

$$\frac{d^2R_{n,l}(r)}{dr^2}+\left[\frac{2\mu}{\hbar^2}E_{n,l}-\frac{1}{b^2}\left(\frac{\alpha(\alpha-1)e^{-2r/b}}{\left(1-e^{r/b}\right)^2}-\frac{\beta e^{-r/b}}{1-e^{-r/b}}\right)-\frac{l(l+1)}{r^2}\right]R_{n,l}(r)=0 \tag{10}$$

Due to the presence of the centrifugal term, Eq. (10) can only be solved analytically for $l\neq 0$. Therefore, we employ an approximation scheme to deal with the centrifugal barrier (Greene and Aldrich, 1976; Qiang and Dong, 2009).

$$\frac{1}{r^2}\approx\frac{1}{b^2}\frac{e^{-r/b}}{\left(1-e^{-r/b}\right)^2} \tag{11}$$

To solve by the present method we need to recast Eq. (10) into the form of Eq. (3) by making changes of variables $r\to z$, through the mapping function and energy transformation.

$$z=e^{-r/b},\quad \varepsilon^2=-\frac{2\mu\hbar^2E_{nl}}{\hbar^2} \tag{12}$$

The hyper geometric equation becomes

$$\frac{d^2R(z)}{dz^2}+\frac{1-z}{z(1-z)}\frac{dR(z)}{dz}+\frac{1}{z^2(1-z)^2}\begin{bmatrix}-\varepsilon^2+\left(\beta+2\varepsilon^2-l(l+1)\right)z\\-\left(\beta+\varepsilon^2+\alpha(\alpha-1)\right)z^2\end{bmatrix}R(z)=0 \tag{13}$$

Comparing Eq. (13) with Eq. (3) we deduce the following for the coefficient

$$\begin{aligned}&c_1=c_2=c_3=1,\ \xi_1=\beta+\varepsilon^2+\alpha(\alpha-1),\ \xi_2=\beta+2\varepsilon^2-l(l+1)\\&\xi_3=\varepsilon^2,\ c_4=0,\ c_5=-\tfrac{1}{2},\ c_6=\tfrac{1}{4}+\beta+\varepsilon^2+\alpha(\alpha-1),\\&c_7=l(l+1)-2\varepsilon^2-\beta, c_8=\varepsilon^2,\ c_9=\tfrac{1}{4}+\alpha(\alpha-1)+l(l+1),\\&c_{10}=1+2\varepsilon,\ c_{11}=2+2\left(\sqrt{\alpha(\alpha-1)+\left(l+\tfrac{1}{2}\right)^2}\right)+2\varepsilon\\&c_{12}=\varepsilon,\ c_{13}=-\tfrac{1}{2}-\left(\sqrt{\alpha(\alpha-1)+\left(l+\tfrac{1}{2}\right)^2}+\varepsilon\right)s\end{aligned} \tag{14}$$

Substituting the parameters, we obtain the energy eigen value and corresponding wave function for modified Manning-Rosen potential as

$$E_{nl}=\frac{-\hbar^2}{2\mu b^2}\left[\frac{\left(n^2+n+\frac{1}{2}\right)+(2n+1)\sqrt{\alpha(\alpha-1)+\left(l+\frac{1}{2}\right)^2}+l(l+1)-\beta}{(2n+1)+2\sqrt{\alpha(\alpha-1)+\left(l+\frac{1}{2}\right)^2}}\right] \tag{15}$$

$$R(z)=N_{n,l}z^{\varepsilon}(1-z)^{-\varepsilon-\frac{1}{2}-\wedge}P_n^{(2\varepsilon,2\wedge+1)}(1-2z) \tag{16}$$

where N_{nl} is the unnormalized constant.

$$\wedge=\sqrt{\alpha(\alpha-1)+\left(l+\tfrac{1}{2}\right)^2} \tag{17}$$

Shannon Entropy and Information Energy of modified Manning-Rosen potential

Here, we write the radial wave function in exponential form and obtain the normalization constants

$$R_{nl}(r)=N_{nl}e^{-\frac{r}{b}}\left(1-e^{-\frac{r}{b}}\right)^{-\varepsilon+\frac{1}{2}+\wedge}P_n^{(2\varepsilon,2\wedge+l)}\left(1-e^{-\frac{r}{b}}\right) \tag{18}$$

The wave functions satisfy, the normalization condition

$$\int_0^{\infty} \left|R_{nl}(r)\right|^2 dr = 1 = b\int_0^1 z^{-1}\left|R_{nl}(z)\right|^2 dz \tag{19}$$

where N_{nl} can be determined through

$$1 = bN_{nl}^2 \int_0^1 z^{2\varepsilon-1}(1-z)^{2\varepsilon+2\wedge-1}\left[P_n^{(2\varepsilon,2\wedge+1)}(1-2z)\right]^2 dz. \tag{20}$$

This equation satisfies the requirements $R_{nl}(z)=0$ as $z=0\ (r\to\infty)$ and $R_{nl}(z)=0$ as $z=1(r\to 0)$.Therefore, the wave function in Eq, (16) are valid physically in the closed interval $z=[0,1]$ as $r=(0,\infty)$. Using the following integral representation of hyper geometric functions (Falaye *et al.*, 2014 and Onate *et al.*, 2017)

$$2F_1(\alpha_0,\beta_0,\gamma_0,1)\frac{\Gamma(\alpha_0)\Gamma(\gamma_0-\alpha_0)}{\Gamma(\gamma_0)} = \int_0^1 z^{\alpha_0-1}(1-z)^{\gamma_0-\alpha_0-1}(1-z)^{-\beta_0} dz \tag{21}$$

gives

$$\frac{{}_2F_1(\alpha_0,\beta_0:\alpha_0+1:1)}{\alpha_0} = \int_0^1 z^{\alpha_0-1}(1-z)^{-\beta_0} dz \tag{22}$$

where

$${}_2F_1(\alpha_0,\beta_0:\gamma_2:1) = \frac{\Gamma(\gamma_0)\Gamma(\gamma_0-\alpha_0-\beta_0)}{\Gamma(\gamma_0-\alpha_0)\Gamma(\gamma_0-\beta_0)} \tag{23}$$

The normalized constant becomes

$$N_{nl} = \frac{1}{\sqrt{z(n)}} \tag{24}$$

$$z(n) = b(-1)^n \frac{\Gamma(n+2\wedge+2)\Gamma(n+2\varepsilon+1)^2}{\Gamma(n+2\varepsilon+2\wedge+2)}\times$$
$$\sum_{p,\gamma=0}^{n} \frac{(-1)^{p+\gamma}\Gamma(n+2\varepsilon+\gamma-p+1)(p+2\wedge+2)}{p!\gamma!(n-p)!(n-\gamma)!\Gamma(n+2\varepsilon-p+1)\Gamma(2\varepsilon+\gamma+1)(n+2\varepsilon+\gamma+2\wedge+2)} \tag{25}$$

Shannon Entropy

In any quantum mechanical system, the Shannon entropy is the logarithmic function of the density which has application in various areas of sciences. It is mathematically obtained as (Shannon, 1948 and Onate *et al.*, 2017)

$$S(\gamma) = -4\pi\int_0^{\infty} \gamma(p)\ln\gamma(p)dp,\ \gamma(p) = R(y)^2 \tag{26}$$

$$S(\gamma) = \frac{b(-1)^n\Gamma(n+2\wedge+2)\Gamma(n+2\varepsilon+1)^2\pi}{\Gamma(n+2\varepsilon+2\wedge+2)}\times$$
$$\ln\gamma(p)\int_{-1}^{1}\left(\tfrac{1-y}{2}\right)^{2\varepsilon-1}\left(\tfrac{1+y}{2}\right)^{2\wedge}\left[P_n^{2\varepsilon,2\wedge+1}\right]^2 dy \tag{27}$$

Defining a relationship of the form

$$x^{\alpha}(1-x)^{\beta}\left[P_n^{(\alpha,\beta)}(x)\right] = x^{\alpha}(1-x)^{\beta}\,{}_2F_1(-n,n+2(\alpha+\beta):2\alpha+1,x) \tag{28}$$

$${}_2F_1\left(-n,n+p+q+1;p+1;\tfrac{1-x}{2}\right) = \tfrac{n!}{(p+1)_n}P_n^{(p,q)}(x),\ (p+1)_n = \frac{\Gamma(n+p+1)}{\Gamma(p+1)} \tag{29}$$

and using integral of the form

$$\int_{-1}^{1}\left(\tfrac{1-x}{2}\right)^{v-1}\left(\tfrac{1+x}{2}\right)^{u}\left[P_n^{(v,u)}(x)\right]^2 dx = \frac{2\Gamma(v+n+1)\Gamma(u+n+1)}{n!v\Gamma(v+u+n+1)} \tag{30}$$

By using Eq. (29) and Eq. (30), the Shannon entropy in Eq. (27) becomes

$$S(\gamma)=\frac{12.568b(2\wedge+1)}{2^{2\wedge+2\varepsilon-1}2}\ln\Big[(0.7844)^{2\varepsilon+1}(0.2156)^{2\wedge}\times$$
$$b(-1)^{n}\frac{(2\wedge+1)\Gamma(n+2\wedge+2)\Gamma(n+2\varepsilon+1)}{2^{2\wedge+2\varepsilon}\Gamma(2\wedge+1)\Gamma(n+2\varepsilon+2\wedge+2)}\tag{31}$$

Information Energy

In any quantum mechanical system, the information energy is mathematically given as (Onate *et al*., 2017)

$$E(\gamma)=4\pi\int_{0}^{\infty}p^{2}\gamma^{2}(p)dp\tag{32}$$

To compute the information energy for easy understanding, we first define a relationship of the form

$$N=4\pi P^{2}\tag{33}$$

So that E(γ) becomes

$$E(\gamma)=N\int_{0}^{\infty}\gamma^{2}(p)dp\tag{34}$$

$$E(\gamma)=N_{1}\int_{-1}^{1}\left[\left(\tfrac{1-y}{2}\right)^{2\varepsilon-1}\left(\tfrac{1+y}{2}\right)^{2\wedge}\left[P_{n}^{2\varepsilon,2\wedge-1}(y)\right]^{2}\right]^{2}dy\tag{35}$$

$$N_{1}=NN_{nl}^{4}$$

Using Eq.(29) and (25), we obtain the information energy as

$$E(\gamma)=1.00544\left(\frac{b(2\wedge+1)}{2^{2\wedge+2\varepsilon}}\right)^{2}\tag{36}$$

RESULTS AND DISCUSSION

In the work, we have utilized the hyper-geometric method and solved the radial SE for the modified Manning-Rosen potential model with the angular momentum $(l\neq 0)$ states. We have derived the binding energy spectra and their corresponding wave functions.

Let us study special cases. We have shown that inserting $\alpha=0$ and $\varepsilon_{0}\beta=V_{0}$ and $\frac{1}{b}=\delta$ in Eq. (1) reduces to the Hulthen potential (Ikot *et al*., 2011)

$$V^{H}(r)=\frac{-V_{0}e^{-\delta r}}{1-e^{-\delta r}}:\ V_{0}=Ze^{2}\delta;\ \delta=b^{-1}\tag{37}$$

where ze^{2} is the potential strength parameter and δ is the screening parameter. We also note that it's possible to recover the Yukawa potential by letting $b\rightarrow\infty$ and $V_{0}=\frac{ze^{2}}{b}$ and the energy for $l\neq 0$ states is

$$E_{nl}=-\frac{[\beta-(n+l+1)]^{2}\hbar^{2}}{8\mu b^{2}(n+l+1)^{2}}\tag{38}$$

and for the s-wave $(l=0)$ states

$$E_{nl}=\frac{-\left[\beta-(n+1)^{2}\right]\hbar^{2}}{8\mu b^{2}(n+1)^{2}}\tag{39}$$

and corresponding radial wave functions are expressed as

$$R_{nl}(r)=N_{nl}e^{-\delta r}\left(1-e^{-\delta r}\right)^{l+1}P_{n}^{(2\varepsilon,2l+1)}\left(1-2e^{-\delta r}\right)\tag{40}$$

We calculate the energy eigenvalues for various n and l quantum numbers with two different values of the parameters α are shown in Table 1. The energy spectra for various diatomic molecules like HCl, LiH and CO are presented in Table 2. These results are relevant in atomic physics, molecular physics and chemical physics.

Table 1: Energy (in atomic units) of different n and l states for $\hbar = 1$

States	$\frac{1}{b}$	α=0.75	α=1.5
2p	0.025	-0.1205	-0.0900
	0.050	-0.1084	-0.0802
	0.075	-0.0969	-0.0710
3p	0.025	-0.0459	-0.0369
	0.050	-0.0352	-0.0274
	0.075	-0.0260	-0.0173
3d	0.025	-0.0449	-0.0396
	0.050	-0.0343	-0.0300
	0.075	-0.0251	-0.0218

Table 2: Energy spectrum of HCl, LiH and CO (ineV) for different states
$Ze = 1973.29eV$, $\mu_{HCl} = 0.9801\,amu$, $\mu_{LiH} = 0.8801\,amu$ and $\mu_{CO} = 6.8606\,amu$, $\hbar = 1$

States	$\frac{1}{b}$	α=0.1		
		HCl	LiH	CO
2p	0.025	-4.8115	-5.3581	-1.3747
	0.050	-4.3183	-4.8089	-1.2338
	0.075	-3.8518	-4.2894	-1.1005
3p	0.025	-1.8663	-2.0783	-0.5332
	0.050	-1.4231	-1.5848	-0.4066
	0.075	-1.0399	-1.1581	-0.2971
3d	0.025	-1.8663	-2.0783	-0.5332
	0.050	-1.4231	-1.5848	-0.4066
	0.075	-1.0399	-1.1561	-0.2991

CONCLUSION

The approximate solutions for the l-wave Schrödinger equation with the modified Manning-Rosen potential has been presented by making a proper approximation to the centrifugal term. The radial wave function and corresponding eigenvalues of the potential is obtained. Some basic theoretical quantities such as the Shannon energy and Information energy under the modified Manning-Rosen potential are also obtained. We have shown that for $\alpha = 0$, the present solution reduces to the one of Hulthen potential. We note that it's possible to recover the Yukawa potential by letting $b \to \infty$. Obviously, the results are in good agreement with those obtained by other methods for short potential range. We have also studied two special cases for $l = 0$ and $l \neq 0$ for the Hulthen potential and presented numerical results of the energy eigenvalues for modified Manning-Rosen potential for different values of n and l states. For further application of our work, we compute energy spectra for different molecules such as HCl, LiH and CO.

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