Approximate Ro-Vibrational Spectrum of the Modified Rosen–Morse Molecular Potential Using the Nikiforov–Uvarov Method

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By using the Nikiforov–Uvarov (NU) method and a new approximation scheme to the centrifugal term, we obtained the solutions of the radial Schrödinger equation (SE) for the modified Rosen–Morse (mRM) potential. In this paper, we get the approximate energy eigenvalues and show that the results are in good agreement with those obtained before. Eigenfunctions are also presented for completeness.

Key words: Schrödinger Equation; Modified Rosen–Morse Potential; Nikiforov–Uvarov Method.
PACS numbers: 03.65.-w; 04.20.Jb; 03.65.Fd; 02.30.Gp

1. Introduction

In many fields of physics and chemistry, explicit analytical solutions of the fundamental dynamical equations are much valuable for a general understanding of phenomena, e.g. the role played by physical parameters. Two typical examples in quantum mechanics are the exact solutions of the Schrödinger equation (SE) for a hydrogen atom (Coulombic) and for a harmonic oscillator [1 – 3]. The Mie-type and pseudoharmonic potentials are also two exactly solvable potentials [4, 5]. Further, there are many potentials that are exactly solvable for zero angular momentum (i. e. $l = 0$). However, their analytic exact solutions can not be obtained for $l \neq 0$, and many authors have used various approximation schemes to solve these problems [6 – 23].

The modified Rosen–Morse potential (also called Scarf II type) [24, 25] is an exponential and anharmonic potential defined by

$$V_{\mathrm{mRM}}(r) = \frac{V_1 - V_2 \sinh(\alpha r)}{\cosh^2(\alpha r)} \tag{1}$$
$$= V_1 \operatorname{sech}^2(\alpha r) - V_2 \operatorname{sech}(\alpha r) \tanh(\alpha r),$$

where $r \in (0, \infty)$; V_1 and V_2 determine the depth of the potential, and $1/\alpha$ denotes the range of the potential well. On the other hand, the Rosen–Morse (RM) potential has the form $V_{\mathrm{RM}}(r) = V_1 \operatorname{sech}^2(\alpha r) - V_2 \tanh(\alpha r)$ and is useful for describing interatomic interaction of linear molecules and helpful for discussing polyatomic vibration energies such as the vibration states of a NH_3 molecule [26, 27]. Additionally, for the avoidance of doubt, we note that the form of the second Pöschl–Teller potential is $V(r) = V_1 - V_2 \cosh(\alpha r)(\sinh^2(\alpha r))^{-1}$ [28].

By taking a proper approximation to the centrifugal term, Qiang and Dong presented arbitrary l-state solutions of the Schrödinger equation with Scarf II potential [29]. Gu et al. calculated the energy spectrum of the Schrödinger equation with the modified Rosen–Morse potential by exact quantization rule [30]. Motavalli and Akbarieh presented the exact solutions of the one-dimensional Klein–Gordon equation for the Scarf-type potential with equal scalar and vector potentials using the Nikiforov–Uvarov (NU) method [31]. By applying a Pekeris-type approximation to the centrifugal term, Chen and Wei studied the spin symmetry of a Dirac nucleon subjected to scalar and vector mRM potentials [32]. Also, Wei and Dong examined the pseudospin symmetry case subjected to the mRM potential [33, 34]. Very recently, Qiang et al. presented the real exact solutions to a relativistic spinless particle with modified Rosen–Morse potential and also for its parity–time (PT) symmetry [35].

The aim of this work is to obtain the approximate bound state energy eigenvalue equation and the corresponding unnormalized wave function of the mRM potential using the new approximation scheme to the centrifugal term [29, 32, 33] and also the concepts of the NU method [36 − 41].

The structure of the paper is as follows: in Section 2, the NU method is briefly introduced. In Section 3, we solve the SE and give energy spectra and corresponding wave functions. Some numerical results are given in this section too. Finally, the relevant conclusions are given in Section 4.

2. Nikiforov–Uvarov Method

The NU method can be used to solve second-order differential equations with an appropriate coordinate transformation $s = s(r)$ [36]:

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0, \qquad (2)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. A solution of (2) is found by a separation of variables, using the transformation $\psi_n(s) = \phi(s)y_n(s)$. It reduces to an equation of the hypergeometric type,

$$\sigma(s)y_n''(s) + \tau(s)y_n'(s) + \lambda y_n(s) = 0. \qquad (3)$$

$y_n(s)$ is the hypergeometric-type function whose polynomials solutions are given by the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)}\frac{\mathrm{d}^n}{\mathrm{d}s^n}\left[\sigma^n(s)\rho(s)\right], \qquad (4)$$

where B_n is the normalization constant and the weight function $\rho(s)$ must satisfy the condition

$$\frac{\mathrm{d}}{\mathrm{d}s}\sigma(s)\rho(s) = \tau(s)\rho(s). \qquad (5)$$

$\phi(s)$ is defined from its logarithmic derivative relation:

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}. \qquad (6)$$

The function $\pi(s)$ and the parameter λ, required for this method, are defined as

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \quad (7a)$$

$$\lambda = k + \pi'(s). \qquad (7b)$$

In order to find the value of k, the expression under the square root must be a square of a polynomial. Thus, a new eigenvalue equation is

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \qquad (8)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \qquad (9)$$

and its derivative must be negative [37 − 41].

3. Solution of Radial Schrödinger Equation with the modified Rosen–Morse Potential

To study any quantum physical system characterized by the empirical potential given in (1), we solve the original SE which is given in well-known textbooks [1, 2]:

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\psi(r, \theta, \varphi) = E\psi(r, \theta, \varphi), \qquad (10)$$

where the potential $V(r)$ is taken as mRM potential form in (1), μ is the reduced mass, and ∇^2 is the Laplacian operator. Using the Laplacian operator in spherical coordinates and decomposing the wave function as $\psi(r, \theta, \varphi) = \frac{R(r)}{r}Y_{lm}(\theta, \varphi)$ [9], we obtain the following radial SE in natural units $\hbar = \mu = 1$:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + 2\left(E_{nl} - \frac{V_1 - V_2\sinh(\alpha r)}{\cosh^2(\alpha r)}\right) - \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0. \qquad (11)$$

Because of the centrifugal term, (11) cannot be solved analytically for $l \neq 0$. Therefore, we attempt to use an approximation scheme to deal with the centrifugal term. To do this, we use a transformation $z = \sinh(\alpha r)$ so that the above equation reduces to

$$\left[\alpha^2(1 + z^2)\frac{\mathrm{d}^2}{\mathrm{d}z^2} + \alpha^2 z\frac{\mathrm{d}}{\mathrm{d}z} + 2\left(E_{nl} - \frac{V_1 - V_2 z}{1 + z^2}\right) - \frac{l(l+1)}{\mathrm{arcsinh}^2(z)}\right]R_{nl}(z) = 0. \qquad (12)$$

Using the definition of $\frac{\mathrm{d}V_{\mathrm{mRM}}(z)}{\mathrm{d}z}\Big|_{z=z_0} = \frac{V_2 z^2 - 2V_1 z - V_2}{(1+z^2)^2}\Big|_{z=z_0} = 0$, we obtain the minimum of the

mRM potential at $z_0 = \left(V_1 + \sqrt{V_1^2 + V_2^2}\right)\Big/ V_2$ or at $r_0 = \frac{1}{\alpha}\sinh^{-1}\left(\left(V_1 + \sqrt{V_1^2 + V_2^2}\right)\Big/ V_2\right)$ [29, 32, 33] and also

$$\frac{d^2V(r)}{dr^2}\bigg|_{r=r_0} = \frac{8(V_0+V_1)(V_0+V_1+V_2)}{V_2^2 V_{12}^3} \\ - \frac{3V_1+2V_0}{V_{12}^2} \tag{13}$$

and

$$V(r_0) = -\frac{V_2^2 V_0}{V_{12}} = -\frac{V_2^2\sqrt{V_1^2+V_2^2}}{V_2^2+\left(V_1+\sqrt{V_1^2+V_2^2}\right)^2}, \tag{14}$$

where $V_0 = \sqrt{V_1^2+V_2^2}$ and $V_{12} = V_2^2 + \left(V_1 + \sqrt{V_1^2+V_2^2}\right)^2$. Now, we expand the centrifugal potential around $z = z_0$ as

$$V_l(r) = \frac{l(l+1)}{\operatorname{arcsinh}^2(z)} \cong l(l+1)\left[\frac{1}{\operatorname{arcsinh}^2(z_0)}\right. \\ - \frac{2(z-z_0)}{\sqrt{1+z_0^2}\operatorname{arcsinh}^3(z_0)} + \left(\frac{3}{(1+z_0^2)\operatorname{arcsinh}^4(z_0)}\right. \\ \left.\left. + \frac{z_0}{(1+z_0^2)^{3/2}\operatorname{arcsinh}^3(z_0)}\right)(z-z_0)^2 + O(z-z_0)^3\right]. \tag{15}$$

Further, the following form of the potential can be used instead of the centrifugal potential in the approximation:

$$\tilde{V}_l(r) = l(l+1)\frac{c_0 + c_1 z + c_2 z^2}{1+z^2}. \tag{16}$$

By expanding the right hand side of (16) up to the terms z^2, then, the resulting equation after a little algebra is compared with (15). The relations between the coefficients and parameters z_0 are obtained as follows:

$$c_0 = \frac{3z_0^2}{\operatorname{arcsinh}^4(z_0)} - \frac{z_0\left(z_0^2-2\right)}{\sqrt{z_0^2+1}\operatorname{arcsinh}^3(z_0)} \\ + \frac{1}{\operatorname{arcsinh}^2(z_0)}, \tag{17a}$$

$$c_1 = -2\left(\frac{1-2z_0^2}{\sqrt{z_0^2+1}\operatorname{arcsinh}^3(z_0)} + \frac{3z_0}{\operatorname{arcsinh}^4(z_0)}\right) \tag{17b}$$

$$c_2 = \frac{3}{\operatorname{arcsinh}^4(z_0)} - \frac{3z_0}{\sqrt{z_0^2+1}\operatorname{arcsinh}^3(z_0)} \\ + \frac{1}{\operatorname{arcsinh}^2(z_0)}. \tag{17c}$$

It must be noted that the approximate scheme $1/r^2 \approx \alpha^2 e^{-\alpha r}/(1-e^{-\alpha r})^2$ used previously for a few potentials [42, 43] is unsuitable for the mRM potential and makes the present quantum system unsolvable.

Now, we can take the potential $\tilde{V}_l$ (16) instead of the centrifugal potential (15) [29]. Hence, by introducing the new variable $s = iz$, (12) reduces to

$$\left[\frac{d^2}{ds^2} + \frac{-s}{1-s^2}\frac{d}{ds} + \frac{1}{(1-s^2)^2}\left(\varepsilon^2(1-s^2)\right.\right. \\ \left.\left. + i\gamma^2 s + \beta^2\right)\right]R_{nl}(s) = 0, \tag{18}$$

where

$$\varepsilon^2 = c_2 l(l+1) - \frac{2E_{nl}}{\alpha^2}, \tag{19a}$$

$$\gamma^2 = -c_1 l(l+1) + \frac{2V_2}{\alpha^2}, \tag{19b}$$

$$\beta^2 = (c_0 - c_2)l(l+1) + \frac{2V_1}{\alpha^2}. \tag{19c}$$

By comparing (18) and (2), we define the following associated polynomials:

$$\tilde{\tau}(s) = -s, \quad \sigma(s) = 1 - s^2, \\ \tilde{\sigma}(s) = \varepsilon^2(1-s^2) + i\gamma^2 s + \beta^2. \tag{20}$$

Using (7a), $\pi(s)$ is found as

$$\pi(s) = \begin{cases} \frac{s}{2} \pm \left(\sqrt{A_+}s - B_+\right) \\ \quad \text{for } k = \varepsilon^2 - \frac{1}{8}\left(-(4\beta^2+1)\right. \\ \qquad \left. + \sqrt{(1-4\beta^2)^2 + 16\gamma^4}\right), \\ \frac{1}{2} \pm \left(\sqrt{A_-}s - B_-\right) \\ \quad \text{for } k = \varepsilon^2 - \frac{1}{8}\left(-(4\beta^2+1)\right. \\ \qquad \left. - \sqrt{(1-4\beta^2)^2 + 16\gamma^4}\right), \end{cases} \tag{21}$$

where

$$A_\pm = \frac{1}{8}\left(1 - 4\beta^2 \pm \sqrt{(1-4\beta^2)^2 + 16\gamma^4}\right), \tag{22a}$$

$$B_\pm = \sqrt{2}\gamma^2\left(4\beta^2 - 1 \mp \sqrt{(1-4\beta^2)^2 + 16\gamma^4}\right)^{-\frac{1}{2}}. \tag{22b}$$

Table 1. Ro-vibrational spectra (in atomic units) of mRM potential.

State	α	$V_1 = 4, V_2 = 2$			$V_1 = 10, V_2 = 6$		
		NU	Ref. [29]	Ref. [44]	NU	Ref. [29]	Ref. [44]
2p	0.05	−0.218770554	−0.218692	−0.218693	−0.798533916	−0.798438	−0.798435
	0.10	−0.201290457	−0.200976	−0.200977	−0.765770755	−0.765388	−0.765392
	0.15	−0.183715658	−0.183008	−0.183018	−0.732714180	−0.731854	−0.731854
	0.20	−0.166138820	−0.164880	−0.164906	−0.699418175	−0.697889	−0.697895
	0.25	−0.148656744	−0.146690	−0.146763	−0.665938776	−0.663549	−0.663570
	0.30	−0.131369772	−0.128538	−0.128696	−0.632333931	−0.628893	−0.628941
3p	0.05	−0.186941164	−0.186863	−0.186863	−0.736592560	−0.736497	−0.736500
	0.10	−0.142791625	−0.142477	−0.142490	−0.646984396	−0.646602	−0.646610
	0.15	−0.103866478	−0.103159	−0.103245	−0.562275289	−0.561415	−0.561451
	0.20	−0.070415934	−0.069157	−0.069439	−0.482614853	−0.481085	−0.481190
	0.25	−0.042691965	−0.040726	−0.041454	−0.408154046	−0.405764	−0.406025
	0.30	−0.020946946	−0.018115	−0.019741	−0.339044778	−0.335603	−0.336155
3d	0.05	−0.217955225	−0.217641	−0.217640	−0.797583014	−0.797201	−0.797199
	0.10	−0.198164548	−0.196906	−0.196911	−0.762045621	−0.760516	−0.760517
	0.15	−0.177019750	−0.174188	−0.174221	−0.724524532	−0.721083	−0.721096
	0.20	−0.154887442	−0.149853	−0.149975	−0.685225778	−0.679108	−0.679142
	0.25	−0.132168316	−0.124303	−0.124645	−0.644374405	−0.634815	−0.634914
	0.30	−0.109287151	−0.097961	−0.098766	−0.602211934	−0.588447	−0.588680
4p	0.05	−0.157611774	−0.157533	−0.157536	−0.677151203	−0.677056	−0.677059
	0.10	−0.094292793	−0.093978	−0.094021	−0.538198038	−0.537816	−0.537830
	0.15	−0.046517298	−0.045809	−0.046055	−0.414336397	−0.413476	−0.413570
	0.20	−0.014693048	−0.013435	−0.014301	−0.305811532	−0.304282	−0.304585
4d	0.05	−0.186181557	−0.185867	−0.185871	−0.735675505	−0.735293	−0.735294
	0.10	−0.140110000	−0.138851	−0.138905	−0.643529600	−0.642000	−0.642017
	0.15	−0.098661710	−0.095830	−0.096111	−0.554995567	−0.551554	−0.551662
	0.20	−0.062671771	−0.057638	−0.058605	−0.470571179	−0.464453	−0.464802
4f	0.05	−0.216775495	−0.216068	−0.216068	−0.796206218	−0.795346	−0.795345
	0.10	−0.193694199	−0.190863	−0.190876	−0.756676890	−0.753236	−0.753239
	0.15	−0.167628045	−0.161257	−0.161350	−0.712808039	−0.705065	−0.705097
	0.20	−0.139538142	−0.128212	−0.128582	−0.665126887	−0.651361	−0.651470
5p	0.10	−0.055793960	−0.055479	−0.055576	−0.439411679	−0.439029	−0.439068
5d	0.10	−0.092055452	−0.090797	−0.090939	−0.535013580	−0.533484	−0.533543
5f	0.10	−0.136302199	−0.133471	−0.133587	−0.638565233	−0.635124	−0.635166
5g	0.10	−0.187950994	−0.182917	−0.182949	−0.749697519	−0.743580	−0.743587
6p	0.10	−0.027295128	−0.026981	−0.027142	−0.350625321	−0.350243	−0.350300
6d	0.10	−0.054000903	−0.052742	−0.053036	−0.436497559	−0.434968	−0.435078
6f	0.10	−0.088910200	−0.086079	−0.086391	−0.530453575	−0.527012	−0.527126
6g	0.10	−0.131435223	−0.126401	−0.126621	−0.632122888	−0.626005	−0.626087

After finding these four values, we choose a set of them which gives a $\tau(s)$ function (see (9)) with negative derivative. The set of functions is

$$k = \varepsilon^2 - \frac{1}{8}\left(-(4\beta^2 + 1) + \sqrt{(1 - 4\beta^2)^2 + 16\gamma^4}\right),$$

$$\pi(s) = \frac{s}{2} \pm \left(\sqrt{A_+}\,s - B_+\right),$$ (23)

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) = -2\left(1 - \sqrt{A_+}\right)s - 2B_+.$$

From (7b), (8), and the equations above, we obtain

$$\lambda = k + \pi'(s) = \varepsilon^2 - A_+ + \sqrt{A_+} - \frac{1}{4}, \quad (24a)$$

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s)$$
$$= 2n\left(1 - \sqrt{A_+}\right) + n(n-1), \quad (24b)$$

where n is a non-negative integer. By equating right hand side in (24a) and (24b), we get

$$\varepsilon^2 = \frac{1}{4}\left[(2n+1) - 2\sqrt{A_+}\right]^2. \quad (25)$$

Finally, recalling (19) and (22), the energy equation can be obtained as

$$E_{nl} = \frac{\alpha^2 c_2}{2} l(l+1) - \frac{1}{8} \left[2n+1 \right.$$

$$\left. - \frac{1}{\sqrt{2}} \sqrt{1 - 4\beta^2 + \sqrt{(1-4\beta^2)^2 + 16\gamma^4}} \right]^2 \qquad (26)$$

$$= \frac{\alpha^2 c_2}{2} l(l+1) - \frac{1}{8} \left[2n+1 - \frac{1}{\sqrt{2}} \left\{ 1 - 4 \left((c_0 - c_2)l \right. \right. \right.$$

$$\left. \cdot (l+1) + \frac{2V_1}{\alpha^2} \right) + \left\{ \left(1 - 4 \left((c_0 - c_2)l(l+1) + \frac{2V_1}{\alpha^2} \right) \right)^2 \right.$$

$$\left. \left. \left. + 16 \left(-c_1 l(l+1) + \frac{2V_2}{\alpha^2} \right)^2 \right\}^{\frac{1}{2}} \right\}^{\frac{1}{2}} \right]^2$$

which is consistent with [29]. In Table 1, we present the ro-vibrational spectra for mRM potential, with two sets of values for V_1, V_2, and various values of α. As one can see from the table, the approximate results differ very little from the analytical and numerical ones obtained by [29] and [44], respectively.

To find eigenfunctions, we first determine the weight function from (5) as

$$\rho(s) = (1+s)^\mu (1-s)^\eta, \qquad (27)$$

where $\mu = \sqrt{A_+} - B_+$ and $\eta = - \left(\sqrt{A_+} + B_+ \right)$. Substituting (27) into (4), we find the first part of the wave function as

$$y_n(s) = \frac{B_n}{(1+s)^\mu (1-s)^\eta} \frac{d^n}{ds^n} \left[(1+s)^{\mu+n} (1-s)^{\eta+n} \right]$$

$$= B_n P_n^{(\mu,\eta)}(s), \qquad (28)$$

where B_n is the normalization constant and $P_n^{(\mu,\eta)}(s)$ is the Jacobi polynomial. Using (6), we find the other part of the wave function as

$$\phi(s) = (1+s)^\sigma (1-s)^\tau, \qquad (29)$$

where $\sigma = -\frac{\sqrt{A_+} + B_+}{2} + \frac{1}{4}$ and $\tau = \frac{\sqrt{A_+} - B_+}{2} - \frac{1}{4}$. Finally, the radial part of the Schrödinger equation with a mRM potential can be obtained as

$$R_{nl}(s) = \phi(s) y_n(s)$$

$$= N_{nl} (1+s)^\sigma (1-s)^\tau P_n^{(\mu,\eta)}(s), \qquad (30)$$

where N_{nl} is the normalization constant. Note that the substitution of $s = iz = i\sinh(\alpha r)$ makes the radial part of the Schrödinger equation with the mRM potential to include the imaginary part [45].

4. Conclusion

In this paper, we have obtained the bound state solutions of the Schrödinger equation for the modified Rosen–Morse potential in the framework of the Nikiforov–Uvarov method. We have also shown that the energy eigenvalues and corresponding eigenfunctions are in high agreement with those obtained by other analytical and numerical methods.

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