

Approximate solutions of Schrödinger equation for modified Mobius square plus modified Eckart potential

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Abstract: The study presents approximate analytical solutions of the Schrödinger equation for the modified Mobius square plus modified Eckart potential. The energy eigenvalues and corresponding wave functions are obtained using the parametric Nikiforov-Uvarov (NU) method. Special cases of this potential are also reported.

Keywords: Nikiforov-Uvarov Method; Modified Eckart potential, Nikiforov-Uvarov method.

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1 Introduction

Since the inception of quantum mechanics, the solutions of Schrödinger equation and other wave equations for known solvable potentials have attracted enormous interest from many scholars. This is because the solutions contain vital information that is needed to describe a system. However, exact solutions of Schrödinger equation have only been reported in rare cases [14,31,39]. Recently, some authors have tried to solve Schrödinger equation with different potentials [1-9,21,26,36,43,45], using different methods such as Nikiforov-Uvarov (NU) method [33], Path integral [11], Ansatz method [46], supersymmetry technique [12, 17,35], Formular method [20] etc.

Up to now, some authors have tried to solve the Schrödinger equation by combining two or more potentials which can be used for wider range of applications [27]. For

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example, Edet et al. [18] obtained the solutions of Schrödinger equation with a combination of modified Kratzer and Screened Coulomb potential. Also, Edet et al. [19] derived analytical solutions of Schrödinger equation with Hellmann- Kratzer potential model. Ita et al. [28] solved the Schrödinger equation with Manning Rosen and Yukawa potentials. Iyang et al. [29] obtained eigensolutions of N dimensional Schrödinger equation with Varshni- Hulthén potential model. Suparmi et al. [40] investigated the eigensolutions of Schrödinger equation with Woods-Saxon and Eckart potentials.

In the present work, we aim to investigate the solution of Schrödinger equation with modified Mobius square plus modified Eckart potential using the parametric Nikiforov-Uvarov (NU) method.

The modified Mobius square potential is the general form of Hulthén and Morse potentials [10,45]. Many authors have investigated various forms of this potential in relativistic and non-relativistic cases [25,30,37,45]. The modified Mobius square potential takes the form

$$V(r) = -V_o \left(\frac{A + Be^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2, \quad (1)$$

where V_o , A , B , and α are the depth of the potential, the range of the potential, the length of the molecular bond, and adjustable screening parameter, respectively.

The Eckart potential is one of the important exponential potentials with usefulness in physics and chemical physics [9,13,47]. This potential has been studied in literature [22,23,34,41]. The modified Eckart potential takes the form

$$V(r) = V_2 \left[\frac{4e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right] + V_3 \left(\frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right), \quad (2)$$

where V_2 , V_3 , α and q are potential constants. Motivated by the success of the combination of exponential potentials, we attempt to investigate the solutions of Schrödinger equation by the combination of modified Mobius square [eq. (1)] and modified Eckart potential [eq. (2)] via the NU method. The newly proposed potential is of the form

$$V(r) = V_{MMS}(r) + V_{ME}(r) = -V_o \left(\frac{A + Be^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2 + V_2 \left[\frac{4e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right] + V_3 \left(\frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right). \quad (3)$$

Considering the successes in previous studies, we combine the potentials for more application and to allow comparative analysis to existing reports of molecular physics.

The paper is drafted as follows: Section 2 gives a brief review of the NU method. Section 3 presents the solutions of Schrödinger and corresponding wave function with MMSE. In sect. 4, numerical results and special cases are presented. Finally, sect. 5 provides the conclusion.

2 Parametric NU method

The parametric form of the NU method reads [32, 42,47]

$$\frac{d^2\psi(s)}{ds^2} + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \frac{d\psi(s)}{ds} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{s^2(1 - \alpha_3 s)^2} \psi(s) = 0. \quad (4)$$

The energy eigenvalues equation and eigenfunctions respectively satisfy the following equations

$$(\alpha_2 - \alpha_3)n + \alpha_3 n^2 - (2n+1)\alpha_5 + (2n+1)(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) + \alpha_7 + 2\alpha_3\alpha_8 + 2\sqrt{\alpha_8\alpha_9} = 0, \quad (5)$$

$$\psi(s) = N_{nl} s^{\alpha_{12}} (1 - \alpha_3 s)^{-\alpha_{12} - (\alpha_{13}/\alpha_3)} P_n^{(\alpha_{10} - 1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10} - 1)}(1 - 2\alpha_3 s), \quad (6)$$

where,

$$\left. \begin{aligned} \alpha_4 &= \frac{1}{2}(1 - \alpha_1), \alpha_5 = \frac{1}{2}(\alpha_2 - 2\alpha_3), \alpha_6 = \alpha_5^2 + \xi_1, \alpha_7 = 2\alpha_4\alpha_5 - \xi_2, \\ \alpha_8 &= \alpha_4^2 + \xi_3, \alpha_9 = \alpha_3\alpha_7 + \alpha_3^2\alpha_8 + \alpha_6, \alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8}, \\ \alpha_{11} &= \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}), \alpha_{12} = \alpha_4 + \sqrt{\alpha_8}, \alpha_{13} = \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \end{aligned} \right\}, \quad (7)$$

and P_n denotes the orthogonal Jacobi polynomial.

3 Bound state solutions of the Schrödinger equation with modified Mobius square plus modified Eckart potential

Given the radial Schrödinger equation of the form [31]

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2} \right] R_{nl}(r) = 0, \quad (8)$$

where R_{nl} is the radial wave function, μ is the mass, $V(r)$ is the potential function, E_{nl} is the energy, \hbar is the Planck's constant, n is the radial quantum number and l is the orbital angular momentum quantum number. Substituting Eq. (3) into Eq. (8), we obtain

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} \left(E + V_o \left(\frac{A + Be^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2 - V_2 \left[\frac{4e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right] - V_3 \left(\frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right) \right) - \frac{l(l+1)}{r^2} \right] R_{nl}(r) = 0 \quad (9)$$

At this point, we notice that Eq. (9) has no exact solution due to the centrifugal term. Therefore, we use the Greene-Aldrich approximation scheme [24,38,15]

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

Substituting Eq. (10) into Eq. (9) and taking $s = e^{-2\alpha r}$, we have

$$\frac{d^2 R(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR(s)}{ds} + \frac{-\varepsilon^2 s^2 + \gamma s - \varphi}{s^2(1-s)^2} R(s) = 0, \quad (11)$$

where,

$$\varepsilon^2 = \frac{-\mu(E + V_o B^2 + V_3)}{2\alpha^2 \hbar^2}, \quad (12)$$

$$\gamma = \frac{\mu(2ABV_o - 2E - 4V_2)}{2\alpha^2 \hbar^2} - l(l+1), \quad (13)$$

$$\varphi = \frac{-\mu(E + V_o A^2 - V_3)}{2\alpha^2 \hbar^2}. \quad (14)$$

Comparing Eq. (11) with Eq. (9), we obtain values of constants from Eq. (7) as

$$\left. \begin{aligned} \alpha_1 = \alpha_2 = \alpha_3 = 1, \alpha_4 = 0, \alpha_5 = -\frac{1}{2}, \alpha_6 = \varepsilon^2 + \frac{1}{4}, \alpha_7 = -\gamma, \alpha_8 = \varphi, \\ \alpha_9 = \frac{1}{2} \sqrt{(2l+1)^2 - \frac{2\mu(V_o(A+B))^2 - 4V_2}{\alpha^2 \hbar^2}}, \alpha_{10} = 1 + 2\sqrt{\varphi}, \\ \alpha_{11} = 2(1 + \sqrt{\varphi}) + \sqrt{(2l+1)^2 - \frac{2\mu(V_o(A+B))^2 - 4V_2}{\alpha^2 \hbar^2}}, \\ \alpha_{12} = \sqrt{\varphi}, \alpha_{13} = -\frac{1}{2} \left(1 + \sqrt{(2l+1)^2 - \frac{2\mu(V_o(A+B))^2 - 4V_2}{\alpha^2 \hbar^2}} \right) \end{aligned} \right\}. \quad (15)$$

Using Eqs. (15), (5) and (6), we obtain the energy levels and corresponding wave function as

$$E_{nl} = V_3 - A^2 V_o - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{\mu(2V_2 + V_3 - ABV_o - A^2 V_o)}{\alpha^2 \hbar^2} + n(n+1) + \frac{1}{2} + l(l+1) + \left(n + \frac{1}{2} \right) \sqrt{(2l+1)^2 - \frac{2\mu(V_o(A+B))^2 - 4V_2}{\alpha^2 \hbar^2}} \right)^2 \left(1 + 2n + \sqrt{(2l+1)^2 - \frac{2\mu(V_o(A+B))^2 - 4V_2}{\alpha^2 \hbar^2}} \right), \quad (16)$$

and

$$R(s) = N_s \sqrt{\varphi} (1-s) \chi P_n^{(2\sqrt{\varphi}, 2\chi-1)}(1-s), \quad (17)$$

where,

$$\chi = \frac{1}{2} + \frac{1}{2} \sqrt{(2l+1)^2 - \frac{2\mu(V_o(A+B))^2 - 4V_2}{\alpha^2 \hbar^2}}, \quad (18)$$

N is normalization constant.

4 Discussion

Solution of the radial Schrödinger equation for the newly proposed potential derived by superposition of modified Mobius square and modified Eckart potential otherwise known as modified Mobius square-modified Eckart potential (MMSMEP) are obtained within the framework of NU method and a suitable approximation to the centrifugal term. By applying a mathematical software, we obtained numerical results for various energy states with $\alpha = 0.01, 0.02, 0.03$ and 0.04 , as shown in Table 1. It is observed that the energy

increases with as the screening parameter α increases. This implies that energy of the system depends on the screening parameter α .

Fig. 1 is a plot of approximation for the centrifugal term for $\alpha = 0.01$. The plot shows that the approximation is valid for $\alpha \ll 1$. Also, we report the variation of energy states with different parameters of modified Mobius square plus modified Eckart potential as illustrated in Fig.2. It can be seen that the energy increases with increasing values of μ . Also, Fig. 3 shows the behaviour of energy against V_2 . It is seen that the energy increases as V_2 increases and tends to maintain a constant value.

However, Figs 4 and 5 shows variation in energy states versus V_3 and A . From the Figures, it is clear that increasing V_3 leads to an increase in energy while decrease in A leads to an increase in energy.

Figures 6 and 7 show energy variation versus V_0 and α , respectively. It is seen that the energy clearly decreases as V_0 and α increases, in both cases.

4.1 Special cases

Modified Mobius square potential

If $V_2 = V_3 = 0$, Eq.(3) reduces to modified Mobius square potential as

$$V(r) = -V_o \left(\frac{A + Be^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2.$$

(19)

And energy eq. (16) becomes

$$E = -A^2 V_o - \frac{2\alpha^2 \hbar^2}{\mu} \left[\frac{-\frac{\mu V_o A(A+B)}{\alpha^2 \hbar^2} + n(n+1) + \frac{1}{2} + l(l+1) + \left(n + \frac{1}{2}\right) \sqrt{(2l+1)^2 - \frac{2\mu V_o (A+B)^2}{\alpha^2 \hbar^2}}}{1 + 2n + \sqrt{(2l+1)^2 - \frac{2\mu V_o (A+B)^2}{\alpha^2 \hbar^2}}} \right]^2. \quad (20)$$

Eq. (18) is in agreement with Eq. (22) of Ref [37], under the condition $k(k+1) = l(l+1)$.

Eckart potential

If $V_0 = 0$, Eq. (3) reduce to Eckart potential of the form

$$V(r) = V_2 \left[\frac{4e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right] + V_3 \left(\frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right). \quad (21)$$

Eq. (16) becomes

$$E = V_3 - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{\frac{\mu(2V_2 + V_3)}{\alpha^2 \hbar^2} + n(n+1) + \frac{1}{2} + l(l+1) + \left(n + \frac{1}{2}\right) \sqrt{(2l+1)^2 + \frac{8\mu V_2}{\alpha^2 \hbar^2}}}{1 + 2n + \sqrt{(2l+1)^2 + \frac{8\mu V_2}{\alpha^2 \hbar^2}}} \right)^2 \quad (22)$$

Modified Poschl-Teller potential

If we replace $V_0 = V_3 = 0$, then Eq. (3) becomes modified Poschl-Teller potential of the form

$$V(r) = V_2 \left[\frac{4e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right] \quad (23)$$

Eq. (16) reduces to

$$E = - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{\frac{2\mu V_2}{\alpha^2 \hbar^2} + n(n+1) + \frac{1}{2} + l(l+1) + \left(n + \frac{1}{2}\right) \sqrt{(2l+1)^2 + \frac{8\mu V_2}{\alpha^2 \hbar^2}}}{1 + 2n + \sqrt{(2l+1)^2 + \frac{8\mu V_2}{\alpha^2 \hbar^2}}} \right)^2 \quad (24)$$

5 Conclusions

This paper presents an approximate analytical solution of Schrödinger equation for the modified Mobius square plus modified Eckart potential. The energy levels and corresponding wave functions are obtained using the Nikiforov-Uvarov (NU) method. Numerical results of energy are also reported. In addition, special cases of this potential and their respective energy eigenvalues are obtained. From the results, it is observed that the energy increases as the screening parameter α increases. This implies that energy of the system depends on the screening parameter α . The result of the present study is consistent with reports in literature. Our results could be useful in areas of chemical and molecular physics.

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Table 1. Energy eigenvalues of modified Mobius square plus modified Eckart potential with $V_0 = 0.2$, $V_2 = 2$, $V_3 = 0.4$, $B = 0.5$, $A = 1.5$, ($\hbar = \mu = 1$) for various values of $\alpha = 0.01, 0.02, 0.03$ and $\alpha = 0.04$

n	l	$\alpha = 0.01$	$\alpha = 0.02$	$\alpha = 0.03$	$\alpha = 0.04$
0	0	1.965038220	1.974571232	1.984154796	1.993789102
1	0	1.984054306	2.012805596	2.041809960	2.071067940
	1	1.984154794	2.013210742	2.042728718	2.072714028
2	0	2.003171290	2.051443438	2.100372718	2.149959864
	1	2.003272310	2.051852836	2.101305816	2.151639940
	2	2.022389154	2.052671630	2.103171994	2.155000000
3	0	2.022490704	2.090484618	2.159842610	2.230463856
	1	2.022693810	2.090898266	2.160790048	2.232177898
	2	2.022998470	2.091725560	2.162684890	2.235605844
	3	2.041707878	2.092966498	2.165527076	2.240747422
4	0	2.041809960	2.129929004	2.220219224	2.312579000
	1	2.042014128	2.130346902	2.221180992	2.314326988
	2	2.042320382	2.131182690	2.223104486	2.317822782
	3	2.042728716	2.132436368	2.225989622	2.323066016
	4	2.061127444	2.134107912	2.229836276	2.330056144
5	0	2.061230060	2.169776464	2.281502170	2.396304456
	1	2.061435290	2.170198610	2.282478264	2.398086376
	2	2.061743136	2.171042896	2.284430396	2.401649982
	3	2.062153596	2.172309310	2.287358464	2.406994824
	4	2.0621533596	2.173997830	2.291262308	2.414120216
	5	2.062666670	2.176108432	2.296141724	2.423025250

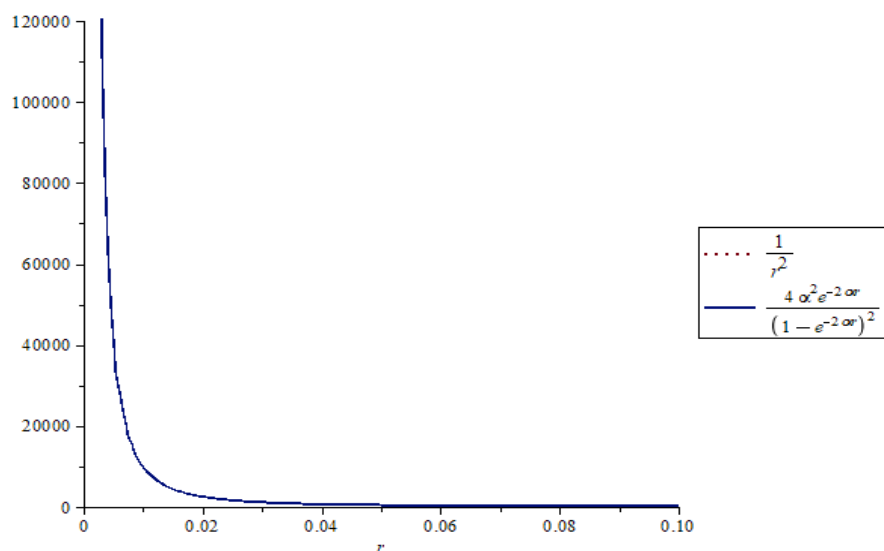


Fig. 1 $\frac{1}{r^2}$ and its approximation scheme for $\alpha = 0.01$

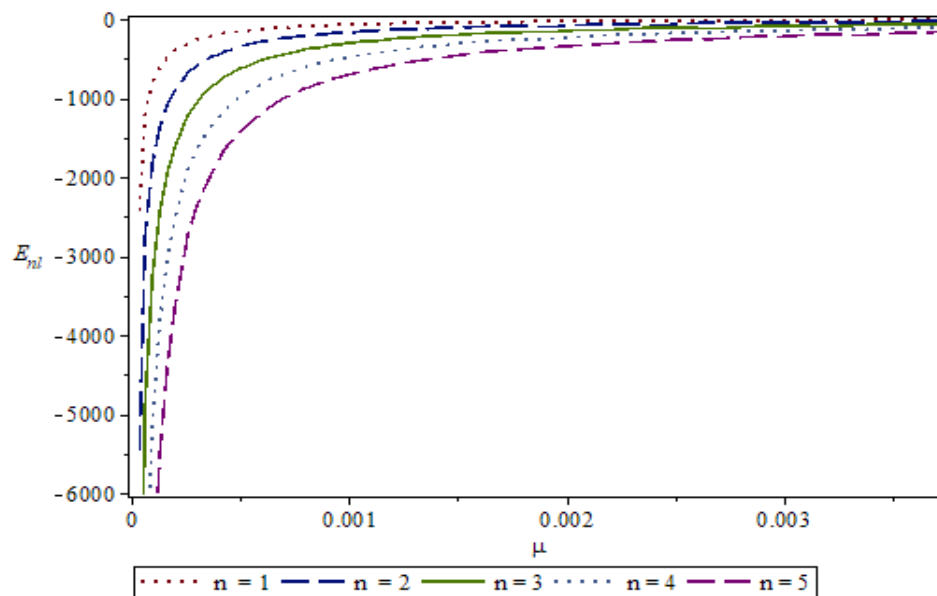


Fig. 2. Energy eigenvalues E_{nl} of modified Mobius squared potential plus modified Eckart potential against μ for various values of n

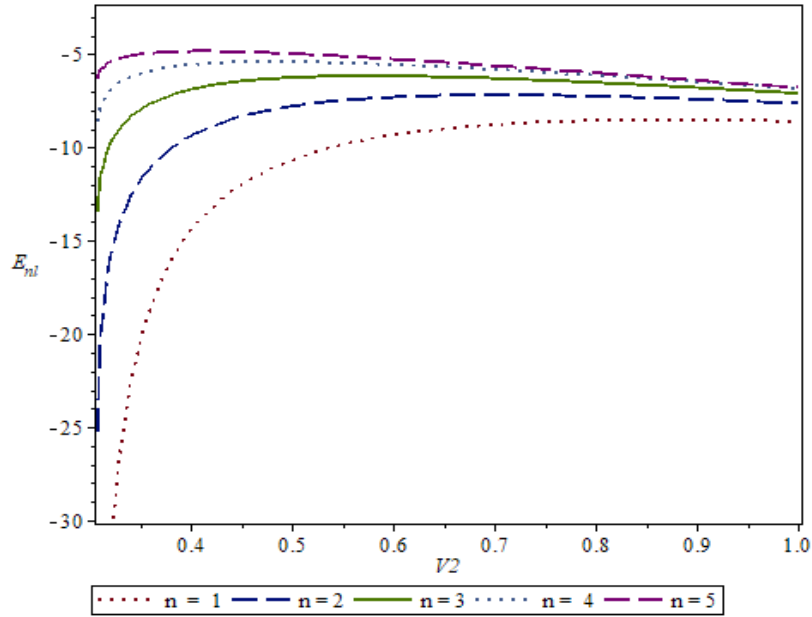


Fig. 3. Energy eigenvalues E_{nl} of modified Mobius squared potential plus modified Eckart potential against V_2 for various values of n

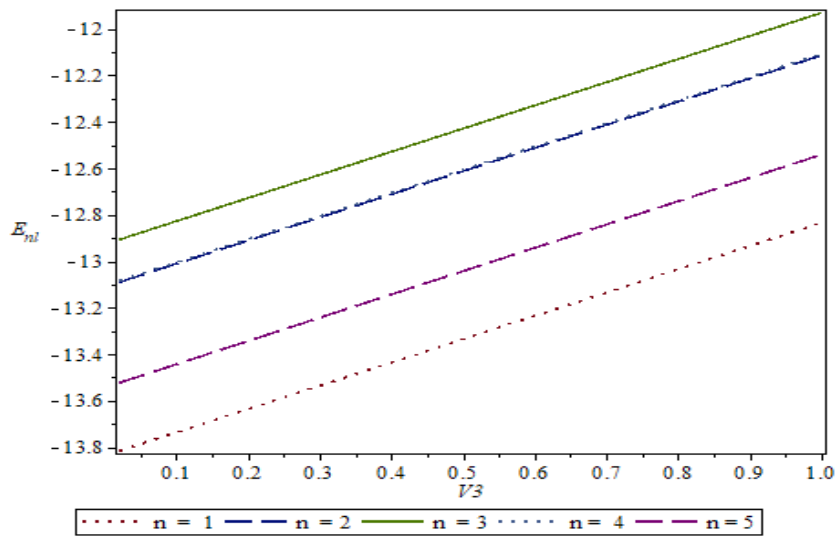


Fig. 4. Energy eigenvalues E_{nl} of modified Mobius squared potential plus modified Eckart potential against V_3 for various values of n

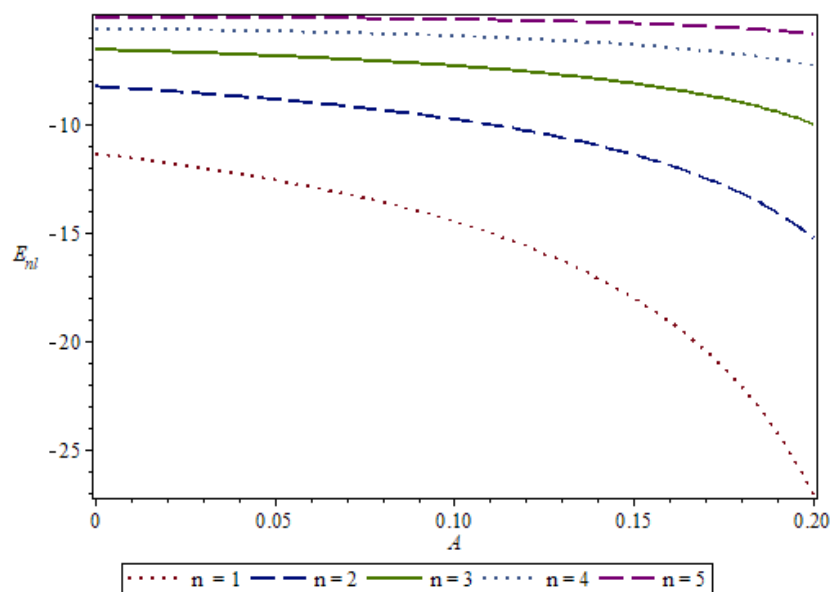


Fig. 5. Energy eigenvalues E_{nl} of modified Mobius squared potential plus modified Eckart potential against A for various values of n

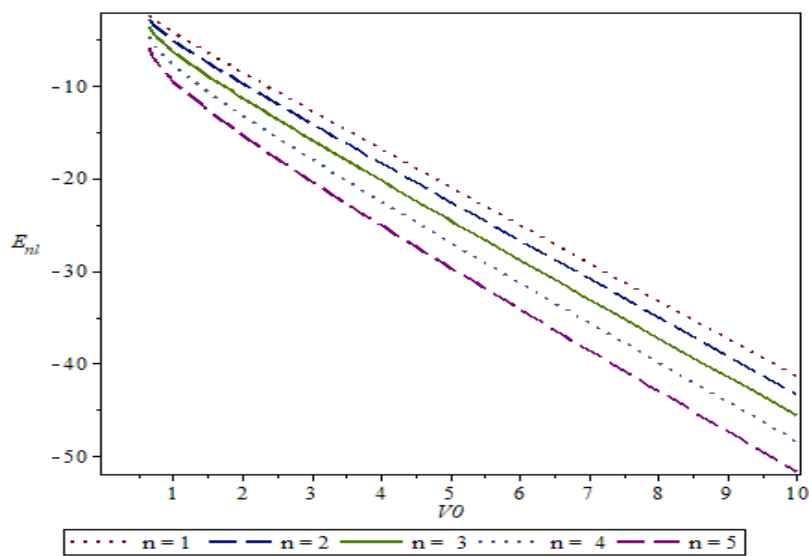


Fig. 6. Energy eigenvalues E_{nl} of modified Mobius squared potential plus modified Eckart potential against V_0 for various values of n

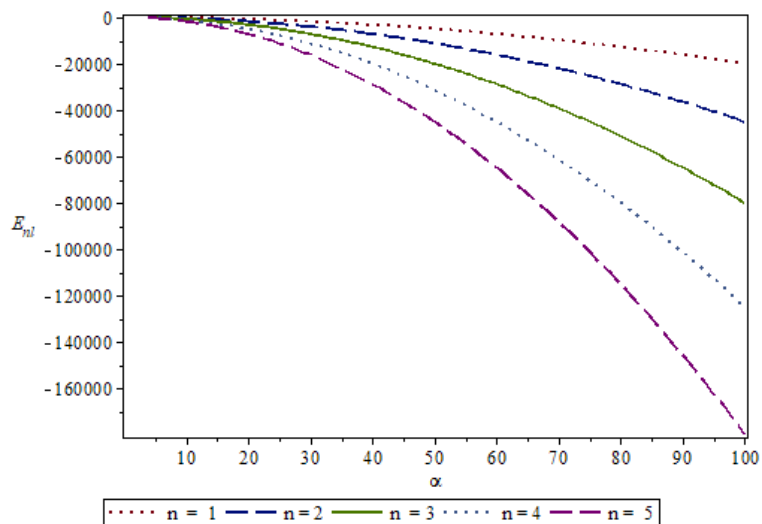


Fig. 7. Energy eigenvalues E_{nl} of modified Mobius squared potential plus modified Eckart potential against α for various values of n