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EXACT SOLUTIONS OF SOLVABLE POTENTIALS WITH SPATIALLY DEPENDENT EFFECTIVE MASSES USING NIKIFOROV-UVAROV METHOD

AKPAN N. IKOT*, LOUIS E. AKPABIO, AKANINYENE D. ANTIA and OLADUNJOYE A. AWOGA

Theoretical Physics Group
Department of Physics
University of Uyo
Nigeria
e-mail: ndemikot2005@yahoo.com

Abstract

We solve the exact solvable potentials of the Schrödinger equation with spatially dependent masses via the Nikiforov-Uvarov method. This method is used to obtain the energy eigenvalues and the corresponding wave functions. As an example, we considered two potentials: (a) Morse potential (b) Singular potential with quadratically growing mass.

1. Introduction

In recent times many authors have studied the Schrödinger equation with different potentials [1-5]. The exact solutions of the Schrödinger equation with position dependent mass have been investigated [6]. These quantum systems with the position dependent effective mass [7] have been investigated for Coulomb-like potential [8], Hardcore potential [9], Harmonic oscillator potential [10], Morse potential [11] and Hulthen potential [12].

An alternative method called the Nikiforov-Uvarov (NU) method [13] has been

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*Corresponding author

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used in recent times for solving the exact solution of the Schrödinger equation [14]. These solutions can be used to get better approximated solutions for potentials more physically interesting [15]. Also many advances have been forwarded in this area by doing the classification of quantum potential regarding its solvability, for instance by relating the solutions to an underlying supersymmetry [16], or a dynamical one [17]. The aim of our study is to analyze the solution of the Schrödinger equation for the mass dependent potential for $l = 0$.

2. Review of Nikiforov-Uvarov Method

The NU-method is based on solving a second order linear differential equation by reducing it to a generalized equation of hypergeometric type [13]. This method has been used to solve the Schrödinger, Dirac and Klein-Gordon equation for different kind of potentials [18]. In NU method, the second order differential equation can be written in the form

$$\psi''(s) + \frac{\overline{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\overline{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \tag{1}$$

where $\sigma(s)$ and $\overline{\sigma}(s)$ are polynomials, at most of second degree and $\overline{\tau}(s)$ is a first degree polynomial. We write the transformation for the wave function in equation (1) as

$$\psi(s) = \varphi(s)\chi_n(s), \tag{2}$$

and equation (1) reduces to equation of hypergeometric type

$$\sigma(s)\chi_n''(s) + \tau(s)\chi_n(s) + \lambda\chi_n(s) = 0, \tag{3}$$

and $\varphi(s)$ is defined as a logarithmic derivative [13]

$$\frac{\varphi'(s)}{\varphi(s)} = \frac{\pi(s)}{\sigma(s)}. \tag{4}$$

The other wave function $\chi_n(s)$ is the hypergoemetric function whose solutions are obtained by the Rodriques relation [13]

$$\chi_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}[\sigma^n(s)\rho(s)], \tag{5}$$

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

$$\frac{d}{ds}(\sigma(s)\rho(s)) = \tau(s)\rho(s). \tag{6}$$

The function $\pi(s)$ in equation (4) and the parameter λ in equation (3) required for the NU-method are defined as follows:

$$\pi(s) = \frac{\sigma' - \bar{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \bar{\tau}}{2}\right) - \bar{\sigma}(s) + k\sigma(s)}, \tag{7}$$

$$\lambda = k + \pi'(s). \tag{8}$$

In order to find value of k in equation (7), then the expression in the square root must be square of a polynomial. Thus, a new eigenvalue equation for the second-order differential equation becomes

$$\lambda = \lambda_n = -\frac{nd\tau(s)}{ds} - \frac{n(n-1)}{2}\frac{d^2\sigma(s)}{ds^2}, \tag{9}$$

where

$$\tau(s) = \bar{\tau}(s) + 2\pi(s) \tag{10}$$

and its derivative is negative. Thus, by the comparison of equation (8), and equation (9), we obtained the energy eigenvalues.

3. Generalized Effective Hamiltonian and the Schrödinger Equation

The general Hermitian effective Hamiltonian for the spatially dependent mass was proposed by Von Roos [19] as

$$H_{VR} = \tfrac{1}{4}[m^{\alpha}(\vec{r})\hat{p}m^{\beta}(\vec{r})m^{\gamma}(\vec{r}) + m^{\gamma}(\vec{r})\hat{p}m^{\beta}(\vec{r})\hat{p}m^{\alpha}(r)], \tag{11}$$

where m is the mass, $\hat{p}$ is the momentum operator α, β and γ are parameters. In order to accommodate the Weyl ordering, Dutra and Almeida [7] use the effective Hamiltonian of the form

$$H = \frac{1}{4(a+1)}[a\{m^{-1}\hat{p}^2 + \hat{p}^2 m^{-1}(r)\}$$

$$+ m^{\alpha}(\vec{r})\hat{p}m^{\beta}(\vec{r})\hat{p}m^{\gamma}(\vec{r}) + m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha}(r)], \tag{12}$$

where a constraint is imposed on the parameter $\alpha + \beta + \gamma = -1$ and the Weyl Ordering is recovered by choosing $a = 1, \alpha = \gamma = 0$ [20].

This effective Hamiltonian can be written as [7]

$$H = \frac{1}{2m}\hat{p}^2 + \frac{i\hbar}{2}\frac{dm/dr}{m^2} + U_{\alpha\beta\gamma\alpha}(r), \tag{13}$$

where

$$U_{\alpha\beta\gamma\alpha}(r) = -\frac{\hbar^2}{4m^3(a+1)}\left[(\alpha+\gamma-a)\frac{md^2m}{dr^2} + 2(a-\alpha\gamma-\alpha-\gamma)\left(\frac{dm}{dr}\right)^2\right]. \tag{14}$$

4. Exact Potentials with Co-ordinate Dependent Mass

The Schrödinger equation with the effective Hamiltonian of equation (13) is written as [7]

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dr^2} + \frac{\hbar^2}{2}\left(\frac{dm/dr}{m^2}\right)\frac{d\psi}{dr} + [V(r) + U_{\alpha\beta\gamma\alpha}(r) - E]\psi = 0. \tag{15}$$

Making the transformation for the wave function as

$$\psi(r) = m^{1/2}(r)R(r). \tag{16}$$

This reduces the Schrödinger equation (15) to the form

$$-\frac{\hbar^2}{2m}\frac{d^2R(r)}{dr^2} + (V_{\text{eff}} - E)R(r) = 0, \tag{17}$$

where the effective potential is defined as

$$V_{\text{eff}} = V(r) + U_{\alpha\beta\gamma\alpha}(r) + \frac{\hbar^2}{4m}\left[3/2\left(\frac{dm/dr}{m}\right)^2 - \frac{1}{m}d^2m/dr^2\right]. \tag{18}$$

4.1. Particular cases

(a) Morse potential

Here $m(r) = m_0 e^{\beta r}$, $V(r) = V_0 e^{\beta r}$. In this case, the effective Schrödinger equation of (17) reduces to

$$\frac{d^2R(r)}{dr^2} + \frac{2m_0}{\hbar^2}[Ee^{\beta r} - V_0 e^{2\beta r} + \varepsilon]R(r) = 0, \tag{19}$$

where $\varepsilon = \hbar^2 / m_0 \left(q - \beta^2 / 8 \right)$ and q is given by

$$q = \beta^2 / 4(a+1) \, (a - 2\alpha\gamma - \alpha - \gamma). \tag{20}$$

We introduce a variable change in equation (19) given as

$$S = e^{\beta r} \tag{21}$$

and it becomes

$$\frac{d^2R}{ds^2} + \frac{1}{s}\frac{dR}{ds} + \frac{1}{s^2}\left[s\overline{E} - \overline{V}_0 s^2 + \overline{\varepsilon}\right]R(s) = 0, \tag{22}$$

where

$$\overline{E} = -\frac{2m_0 E}{\hbar^2\beta^2}, \quad \overline{V_0} = \frac{2m_0 V_0}{\hbar^2\beta^2},$$

$$\overline{\varepsilon} = \frac{2m_0}{\beta^2\hbar^2}\varepsilon. \tag{23}$$

On comparison of equation (22) with equation (1), we obtain the corresponding polynomials as

$$\overline{\tau}(s) = 1, \quad \sigma(s) = s, \quad \overline{\sigma}(s) = -\overline{V}_0 s^2 + s\overline{E} + \overline{\varepsilon}. \tag{24}$$

Substituting this into equation (7), and according to the property that $\pi(s)$ is a polynomial, we find that $\pi(s)$ can take the following four possible values:

$$\pi(s) = \pm\begin{cases} \sqrt{\overline{V}_0}\, s + i\sqrt{\overline{\varepsilon}} \\ \text{for } k = \overline{E} + 2i\sqrt{\overline{\varepsilon}\,\overline{V}_0}, \\ \sqrt{\overline{V}_0}\, s - i\sqrt{\overline{\varepsilon}} \\ \text{for } k = \overline{E} - 2i\sqrt{\overline{\varepsilon}\,\overline{V}_0}, \end{cases} \tag{25}$$

where k is determined by the polynomial $\tau = \overline{\tau} + 2\pi$ having a negative derivative. However, the polynomial $\tau(s)$ in equation (10) for which its derivative has a negative value; is established by a suitable choice of the polynomial $\pi(s)$ for

$k = \overline{E} - 2i\sqrt{\varepsilon\overline{V}_0}$ from equation (25),

$$\pi(s) = -\sqrt{\overline{V}_0}\,s + i\sqrt{\varepsilon},$$
$$\tau(s) = 1 - 2\sqrt{\overline{V}_0}\,s + 2i\sqrt{\varepsilon},$$
$$\tau'(s) = -2\sqrt{\overline{V}_0}.$$

One can easily show that substituting these results into equations (8) and (9) leads to energy eigenvalues

$$E_n = -\hbar\beta\sqrt{\frac{V_0}{2m_0}}\left[1 + 2n + 2i\sqrt{\frac{2m_0\varepsilon}{\hbar^2\beta^2}}\right],\ n = 0, 1, 2, \dots, \tag{27}$$

where we have used equation (23) in obtaining equation (27).

Similarly, the weight function $\rho(s)$ is obtained from equation (6) as

$$\rho(s) = s^{2\mu}e^{-2\upsilon s}, \tag{28}$$

where $\mu = i\sqrt{\overline{\varepsilon}}$ and $\upsilon = \sqrt{\overline{V}_0}$. On substituting equation (28) into the Rodrique relation of equation (5), we get

$$\chi_n(s) = B_n s^{-2\mu}e^{2\upsilon s}\frac{d^n}{ds^n}[s^{n+2\mu}e^{-2\upsilon s}]. \tag{29}$$

Equation (29) can be expressed in terms of Laguerre polynomial as

$$\chi_n(s) = B_n s^{-2\mu}e^{2\upsilon s}L_n^{(2\mu+n)}(s), \tag{30}$$

where B_n is the normalization constant. The other part of the wave function is obtained from equation (4) as

$$\varphi(s) = s^{\mu}e^{-\upsilon s}. \tag{31}$$

Finally, we combine equations (29) and (31) to get the total wave function as

$$R(s) = B_n s^{-\mu}e^{\upsilon s}\frac{d^n}{ds^n}[s^{n+2\mu}e^{-2\upsilon s}]. \tag{32}$$

(b) Singular potential with quadratically growing mass

Here the potential and the effective mass are defined as [7]

$$V(r) = \frac{A}{\beta r^4} + {}^{B}\!/_{\beta r^2}, \quad m(r) = \beta r^2, \tag{33}$$

where A and B are constants.

Substituting equation (33) into the effective Schrödinger equation yields

$$\frac{d^2\psi}{dr^2}+\frac{2}{\hbar}\left[\beta E r^2-\frac{(A+G)}{r^2}-B\right]\psi(r)=0, \tag{34}$$

where $G=\frac{\hbar^2}{2(a+1)}\lfloor 4\alpha\gamma+3(\alpha+\gamma)-a+2\rfloor$. By changing the co-ordinate $r=\beta(1+x)$, we write equation (34) as

$$\frac{d^2\psi}{dx^2}+\frac{2}{\beta^2\hbar^2}\left[\beta^2 E(1+x)^2-\frac{(A+G)}{(1+x)^2}-B\right]\psi(x)=0. \tag{35}$$

The third term in equation (35) can be Taylor expanded as follows

$$\frac{A+G}{(1+x)^2}=\delta[1-2x+3x^2-4x^3+5x^4+\cdots], \tag{36}$$

where $\delta=(A+G)$.

In Pekeris approximation [21], a potential function is defined as [22]

$$V(x)=\delta\left(C_0+\frac{C_1}{1+\exp(\alpha x)}+\frac{C_2}{(1+\exp(\alpha x))^2}\right). \tag{37}$$

If one Taylor expands equation (37), we obtain

$$V(x)=\delta\Bigg[\left(C_0+\frac{C_1}{2}+\frac{C_2}{4}\right)-\alpha/_4(C_1+C_2)x$$

$$+\alpha^2/_{16}C_2x^2+\frac{\alpha^3}{48}(C_1+C_2)x^3-\alpha^4/_{96}C_2x^4+\ldots\Bigg]. \tag{38}$$

Substituting equation (35) into equation (34) and using equations (36)-(37), we obtain

$$\frac{d^2\psi}{dx^2}+\frac{2}{\hbar^2\beta^2}\left[\beta^2 E-\delta C_0-\frac{\delta C_1}{[1+\exp(\alpha x)]}-\frac{\delta C_2}{[1+\exp(\alpha x)]^2}-B\right]\psi(x)=0, \tag{39}$$

where C_0, C_1, and C_2 are arbitrary constants and where the terms in $(1+x)^2$ have been absorbed into the coefficient of the potential term.

Now introducing a new variable $s = -e^{\alpha x}$ and using the following dimensionless parameters,

$$\varepsilon^2 = -\frac{2E}{\hbar^2\beta^2\alpha^2}, \quad \gamma^2 = \frac{2\delta C_0}{\hbar^2\beta^2\alpha^2}, \quad \wedge^2 = \frac{2\delta C_1}{\hbar^2\beta^2\alpha^2},$$

$$\xi^2 = -\frac{2\delta C_2}{\hbar^2\beta^2\alpha^2}, \quad \eta^2 = \frac{2B}{\hbar^2\beta^2\alpha^2}, \tag{40}$$

reduces equation (39) into the generalized hypergeometric type equations as

$$\frac{d^2\psi}{ds^2} + \frac{(1-S)}{S(1-S)}\frac{d\psi}{ds} + \frac{1}{S^2(1-s)^2}[-(\varepsilon^2+\gamma^2+\delta^2)s^2$$

$$+(2\varepsilon^2+2\gamma^2+2\eta^2-\wedge^2)s-(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)]\psi(s)=0. \tag{41}$$

Now comparing equation (41) with equation (1), we have

$$\sigma(s) = s(1-s), \quad \bar{\tau}(s) = (1-s),$$

$$\bar{\sigma}(s) = -as^2 + bs - c, \tag{42}$$

where

$$a = (\varepsilon^2 + \gamma^2 + \eta^2),$$

$$b = (2\varepsilon^2 + 2\gamma^2 + 2\eta^2 + \wedge^2),$$

$$c = (\varepsilon^2 + \gamma^2 + \wedge^2 + \xi^2 + \eta^2). \tag{43}$$

In the NU-method the $\pi(s)$ function is obtained as

$$\pi(s) = -S/2 \pm \frac{1}{2}\sqrt{(1+4a-4k)s^2 + (4k-4b)s + 4c}. \tag{44}$$

The expression in the square root must be the square of a polynomial according to the NU method. Therefore, we can determine the k-value by using condition that the discriminant of the square root is zero, that is,

$$K = -\wedge^2 - 2\xi^2 \pm \sqrt{(4\xi^2+1)(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)}. \tag{45}$$

Using equation (45) in equation (44), we have

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2}\begin{cases} (2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} - \sqrt{4\xi^2+1})s - 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} \\ \text{for } K = -\wedge^2 - 2\xi^2 + \sqrt{(4\xi^2+1)(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)}, \\ \\ (2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} + \sqrt{4\xi^2+1})s - 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} \\ \text{for } K = -\wedge^2 - 2\xi^2 - \sqrt{(4\xi^2+1)(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)}. \end{cases} \tag{46}$$

For the polynomial of $\tau(s) = \bar{\tau}(s) + 2\pi(s)$ which has a negative derivative, we select

$$K = -\wedge^2 - 2\xi^2 - \sqrt{(4\xi^2+1)(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)}$$

and

$$\pi(s) = -\frac{s}{2} - \frac{1}{2}\Big[(2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} + \sqrt{4\xi^2+1})s - 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2}.$$

With this selection, we can obtain $\tau(s)$ from equation (10) as

$$\tau(s) = 1 - 2s - (2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} + \sqrt{4\xi^2+1})s - 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2}, \tag{47}$$

$$\tau'(s) = -2 - 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} - \sqrt{4\xi^2+1}. \tag{48}$$

Applying equations (42) and (47) in equation (9), we have

$$\lambda = \lambda_n = n(2 + 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} - \sqrt{4\xi^2+1}) + n(n-1). \tag{49}$$

Similarly, from equation (8), we have

$$\lambda = -\wedge^2 - 2\xi^2 - \sqrt{(4\xi^2+1)(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)} - \frac{1}{2} - \sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} - \frac{1}{2}\sqrt{4\xi^2+1}. \tag{50}$$

Equating equation (49) to equation (50), we have

$$-\wedge^2 - 2\xi^2 - \sqrt{(4\xi^2+1)(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)} - \frac{1}{2} - \sqrt{(\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2)} - \frac{1}{2}\sqrt{4\xi^2+1} = n(2 + 2\sqrt{\varepsilon^2+\gamma^2+\wedge^2+\xi^2+\eta^2} + \sqrt{4\xi^2+1}) + n(n-1). \tag{51}$$

Solving equation (51) explicitly for ε^2 and substituting in equation (40), we obtain the energy spectrum as

$$E_n = (\delta C_0 + \delta C_1 + \delta C_2 + B) - \frac{\hbar^2\beta^2\alpha^2}{2\left(1 + 2n + \sqrt{\frac{8\delta C_2}{\hbar^2\beta^2\alpha^2} + 1}\right)^2}$$

$$\times\left[\frac{2\delta C_1}{\hbar^2\beta^2\alpha^2} + \frac{4\delta C_2}{\hbar^2\beta^2\alpha^2} + \frac{1}{2} + \frac{1}{2}\sqrt{\frac{8\delta C_2}{\hbar^2\beta^2\alpha^2} + 1} - n - n\sqrt{\frac{8\delta C_2}{\hbar^2\beta^2\alpha^2} + 1} - n^2\right]^2. \quad (52)$$

Similarly, the weight function $\rho(s)$ is obtained from equation (6) as

$$\rho(s) = (1 - s)^{\mu} s^{2\nu}, \quad (53)$$

where $\mu = \sqrt{4\xi^2 + 1}$ and $\nu = \sqrt{\varepsilon^2 + \gamma^2 + \wedge^2 + \xi^2 + \eta^2}$.

On substituting equation (53) into the Rodrique relation of equation (5), we get

$$\chi_n(s) = B_n(1 - s)^{-\mu} S^{-2\upsilon} \frac{d^n}{ds^n}[s^{n+2\upsilon}(1 - s)^{n+\mu}], \quad (54)$$

where B_n is the normalization constant. The other part of the wave function is obtained from equation (4) as

$$\varphi(s) = s^{\upsilon}(1 - s)^{\frac{1}{2}(1+\mu)}. \quad (55)$$

Combining equations (54) and (55), we have the total wave function as

$$\psi(s) = B_n(1 - s)^{\frac{1}{2}(1-\mu)} s^{-\upsilon} \frac{d^n}{ds^n}[s^{n+2\upsilon}(1 - S)^{n+\mu}]. \quad (56)$$

5. Result and Discussion

We plotted the variation of the effective potential V_{eff} with r for the Morse potential in Figure 1 for various parameters of $\beta = -0.5, -1.0, 0.5$ and 1.0. We also plotted the V_{eff} with r for the singular potential with quadratically growing mass for various parameters of $\beta = 1, 2, 3, 4$ and 5 in Figure 2. Choosing the separated atoms limit as the zero of energy, the Morse potential has the form $V(r) = V_0 e^{-\beta r}$, where $V_0 > 0$ corresponds to its depth, β is related to the range of the potential and r is the relative distance from the equilibrium position of the atom. In the limits $\beta \to 0$ and $V_0 \to \infty$, we have [8]

$$\lim_{V_0 \to \infty} V_{\mathrm{Morse}} = \tfrac{1}{2} kr^2,$$

where $k = \beta^2 V_0$.

In the case of the singular potential, our result corresponds to the analytical solution obtained for Woods-Saxon with arbitrary l-value by Badalov et al. [22]. Here the β -values play the analogue role of the arbitrary l-values.

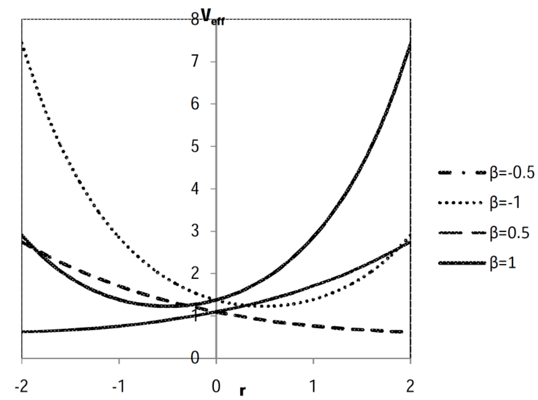

Figure 1. A plot of V_{eff} with r for Morse Potential with various parameters of $\beta = -0.5, -1.0, 0.5$ and 1.0.

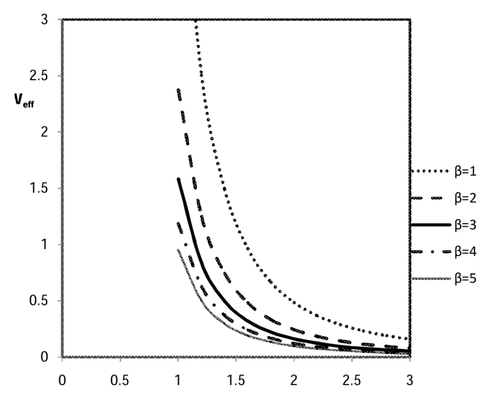

Figure 2. A plot of V_{eff} with r for singular potential and quadratically growing mass with various parameters of $\beta = 1, 2, 3, 4$ and 5.

6. Conclusion

We solve the effective mass Schrodinger equation for Morse potential and the singular potential with quadratic growing mass using Nikiforov-Uvarov method. We obtain the eigenfunction and the corresponding eigenvalues for the two cases.

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