

# A new approach to the exact solutions of the effective mass Schrödinger equation

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## Abstract

Effective mass Schrödinger equation is solved exactly for a given potential. Nikiforov-Uvarov method is used to obtain energy eigenvalues and the corresponding wave functions. A free parameter is used in the transformation of the wave function. The effective mass Schrödinger equation is also solved for the Morse potential transforming to the constant mass Schrödinger equation for a potential. One can also get solution of the effective mass Schrödinger equation starting from the constant mass Schrödinger equation.

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# 1 Introduction

Quantum mechanical systems with spatially dependent effective mass (PDM) has been extensively used in different branch of physics. Special PDM applications can be found in the fields of microstructures such as semiconductors [1], quantum dots [2], helium clusters [3], quantum liquids [4]. Content of the approach requires non-constant mass that depends on position such that the mass and the momentum operator no longer commute in PDM Schrödinger equation [5]. Dekar et al. solved the one dimensional Schrödinger equation with smooth potential and mass step [6]. Fruitful applications have been increased in quantum mechanical problems and various approaches are used in the atomic and nuclear physics and other fields of the physics. Supersymmetric (SUSY) method is very useful technique for exactly solvable potentials that extended to PDM [7]. Several authors have investigated the exact solution of Schrödinger equation with position dependent mass using SUSY techniques [8,9,10].  $so(2,1)$ ,  $su(1,1)$  Lie algebras and quadratic algebra approach for PDM Schrödinger equation in two dimensions were used as generating algebra as a potential algebra to obtain exact solutions of the effective mass wave equation [11,12,13]. Exact solutions of Schrödinger equation in D dimensions, quantum well problem includes PDM approach [14,15] and the point canonical transformations (PCT) are other studies and approaches providing exact solution of energy eigenvalues and corresponding eigenfunctions [16,17,18,19].

Nikiforov-Uvarov approach which received much interest in recent years, has been introduced for solving Schrödinger equation, Klein-Gordon, Dirac and Salpeter equations [20,21,22,23,24,25].

In this work, the PDM Schrödinger equation is solved for a given potential by using the Nikivori-Uvarov method. Energy eigenvalues and the corresponding wave functions are calculated. Then as an application the PDM Schrödinger equation is solved for the Morse potential by transforming into a constant mass Schrödinger equation for a well known potential. It is also shown that solutions of the PDM Schrödinger equation can be obtained starting from the constant mass Schrödinger equation can be obtained for the Morse potential.

The contents of the paper is as follows: in section II, we introduce PDM approach and Nikiforov-Uvarov method. The next section involves applications to Morse potential. Solutions obtained with mass dependent parameters are given in section IV. Results are discussed in section V.

## 2 Method

We write the one-dimensional effective mass Hamiltonian of the SE as [26]

$$H_{eff} = -\frac{d}{dx} \left( \frac{1}{m(x)} \frac{d}{dx} \right) + V_{eff}(x) \quad (1)$$

where  $V_{eff}$  has the form

$$V_{eff} = V(x) + \frac{1}{2}(\beta + 1) \frac{m''}{m^2} - [\alpha(\alpha + \beta + 1) + \beta + 1] \frac{m'}{m^3} \quad (2)$$

with  $\alpha, \beta$  are ambiguity parameters. Primes stand for the derivatives with respect to  $x$ . Thus the SE takes the form

$$\left( -\frac{1}{m} \frac{d^2}{dx^2} + \frac{m'}{m} \frac{d}{dx} + V_{eff} - \varepsilon \right) \varphi(x) = 0 \quad (3)$$

We apply the following transformation

$$\varphi = m^\eta(x) \psi(x) \quad (4)$$

Hence, the SE takes the form

$$\left\{ -\frac{1}{m} \left[ \frac{d^2}{dx^2} + (2\eta - 1) \frac{m'}{m} \frac{d}{dx} + \eta \left( (\eta - 2) \left( \frac{m'}{m} \right)^2 + \frac{m''}{m} \right) \right] + (V_{eff} - \varepsilon) \right\} \psi = 0 \quad (5)$$

For the case of  $\eta = 1/2$ , this equation turns to Eq.(4) in Ref.[26]. Now we assume that

$$m(x) = e^{-2\lambda x} \quad (6)$$

$$V(x) = V_0 e^{2\lambda x} - B(2A + 1)e^{\lambda x} \quad (7)$$

Substituting these relations into Eq.(5), we get

$$-[\psi'' + 2\lambda(2\eta - 1)\psi' + 4\eta\lambda^2(\eta - 1)\psi] + [V_0 - B(2A + 1)e^{-\lambda x} - \varepsilon e^{-2\lambda x} + 2(\beta + 1)\lambda^2 - 4A^*\lambda^2]\psi = 0 \quad (8)$$

where

$$A^* = \alpha(\alpha + \beta + 1) + \beta + 1 \quad (9)$$

The coordinate transformation  $s = e^{-\lambda x}$  leads to

$$\frac{d^2\psi}{ds^2} + (3 - 4\eta)\frac{1}{s}\frac{d\psi}{ds} + \frac{1}{s^2}\left[\frac{\varepsilon}{\lambda^2}s^2 + \frac{1}{\lambda^2}B(2A + 1)s - \frac{V_0}{\lambda^2} - 2(\beta + 1) + 4A^* + 4\eta(\eta - 1)\right]\psi = 0. \quad (10)$$

For simplicity, let us define

$$\xi_1 = -\frac{\varepsilon}{\lambda^2} \quad (11)$$

$$\xi_2 = -\frac{1}{\lambda^2}B(2A + 1) \quad (12)$$

$$-\xi_3 = \frac{V_0}{\lambda^2} + 2(\beta + 1) - 4A^* - 4\eta(\eta + 1) \quad (13)$$

Thus, Eq.(10) has the form

$$\frac{d^2\psi}{ds^2} + (3 - 4\eta)\frac{1}{s}\frac{d\psi}{ds} + \frac{1}{s^2}(-\xi_1 s^2 - \xi_2 s + \xi_3)\psi = 0 \quad (14)$$

Now, we apply the NU method starting from its standard form

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0. \quad (15)$$

Comparing Eqs.(14) and (15), we obtain

$$\sigma = s, \tilde{\tau}(s) = 3 - 4\eta, \tilde{\sigma}(s) = -\xi_1 s^2 - \xi_2 s + \xi_3 \quad (16)$$

where  $\sigma(s)$  and  $\tilde{\sigma}(s)$  are polynomials at most second degree and  $\tilde{\tau}(s)$  is a first-degree polynomial.

In the NU method, the function  $\pi$  and the parameter  $\lambda$  are defined as

$$\pi(s) = \frac{\sigma' - \tau(s)}{2} \pm \sqrt{\left(\frac{\sigma' - \tau(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \quad (17)$$

and

$$\lambda = k + \pi' \quad (18)$$

To find a physical solution, the expression in the square root must be square of a polynomial.

Then, a new eigenvalue equation for the SE becomes

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma''(s), (n = 0, 1, 2, \dots) \quad (19)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \quad (20)$$

and it should have a negative derivative [20]. A family of particular solutions for a given  $\lambda$  has hypergeometric type of degree. Thus,  $\lambda = 0$  will corresponds to energy eigenvalue of the ground state, i.e.  $n = 0$ . The wave function is obtained as a multiple of two independent parts

$$\psi(s) = \phi(s)y(s) \quad (21)$$

where  $y(s)$  is the hypergeometric type function written with a weight function  $\rho$  as

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s) \rho(s)] \quad (22)$$

where  $\rho(s)$  must satisfy the condition [20]

$$(\sigma\rho)' = \tau\rho \quad (23)$$

The other part is defined as a logarithmic derivative

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \quad (24)$$

### 3 Calculations

#### 3.1 Solutions of Eq.(14) with the Nikiforov-Uvarov method

Substituting  $\sigma(s)$ ,  $\tilde{\sigma}$  and  $\tilde{\tau}(s)$  into Eq.(17), we obtain  $\pi$  function as

$$\pi = 2\eta - 1 \pm \sqrt{\xi_1 s^2 - 2Ds + (2\eta - 1)^2 - \xi_3} \quad (25)$$

Due to NU method, the expression in the square root is taken as the square of a polynomial.

Then, one gets the possible functions for each root  $k$  as

$$\pi = 2\eta - 1 \pm \quad (26)$$

$$\begin{cases} \sqrt{\xi_1 s^2 + 2Ds + (2\eta - 1)^2 - \xi_3}, & k_1 = 2\sqrt{\xi_1 [(2\eta - 1)^2 - \xi_3]} - \xi_2; \\ \sqrt{\xi_1 s^2 - 2Ds + (2\eta - 1)^2 - \xi_3}, & k_2 = -2\sqrt{\xi_1 [(2\eta - 1)^2 - \xi_3]} - \xi_2. \end{cases} \quad (27)$$

where  $D^2 = \xi_1 [(2\eta - 1)^2 - \xi_3]$ . From Eq.(20), we obtain  $\tau$  as

$$\tau = \begin{cases} 1 + 2\sqrt{\xi_1} s + \frac{2D}{\sqrt{\xi_1}} \\ 1 - 2\sqrt{\xi_1} s - \frac{2D}{\sqrt{\xi_1}} \\ 1 + 2\sqrt{\xi_1} s - \frac{2D}{\sqrt{\xi_1}} \\ 1 - 2\sqrt{\xi_1} s + \frac{2D}{\sqrt{\xi_1}} \end{cases} \quad (28)$$

Imposing the condition  $\tau' < 0$ , physical solutions are given by two cases:

$$\text{Case I: } k = -\xi_2 + 2D, \pi = 2\eta - 1 - \sqrt{\xi_1}s - \frac{D}{\sqrt{\xi_1}}, \tau = 1 - 2\sqrt{\xi_1}s - \frac{2D}{\sqrt{\xi_1}}$$

From Eq.(19) we obtain energy equation as

$$(2n + 1)\sqrt{\xi_1} = -\xi_2 + 2D \quad (29)$$

Substituting  $\xi_1$ ,  $\xi_2$  and  $D$  in Eq.(9), we solve  $\varepsilon$  as

$$\varepsilon = -\frac{B^2}{\lambda^2}(2A + 1)^2 \left[ 2n + 1 - 2\sqrt{(2\eta - 1)^2 + \frac{V_0}{\lambda^2} + 2(\beta + 1) - 4A^* - 4\eta(\eta - 1)} \right]^{-2} \quad (30)$$

Using  $\sigma(s)$  and  $\pi(s)$  in Eqs.(16) and (26), we obtain the corresponding wave functions  $y(s)$  and  $\phi(s)$ . Then, from Eq.(23) with

$$\rho(s) = s^{-\frac{2D}{\sqrt{\xi_1}}} e^{-2\sqrt{\xi_1}s} \quad (31)$$

we compute  $y_n(s)$  form Eq.(22) as

$$y_n(s) = B_n L_n^{-\frac{2D}{\sqrt{\xi_1}}}(2\sqrt{\xi_1}s) \quad (32)$$

where  $B_n = 1/n!$ . From Eq.(24), we solve

$$\phi(s) = s^{2\eta-1-\frac{D}{\sqrt{\xi_1}}} e^{-\sqrt{\xi_1}s} \quad (33)$$

Thus, total wave function becomes

$$\psi(s) = B_n s^{2\eta-1-\frac{D}{\sqrt{\xi_1}}} e^{-\sqrt{\xi_1}s} L_n^{-\frac{2D}{\sqrt{\xi_1}}}(2\sqrt{\xi_1}s) \quad (34)$$

$$\text{Case II: } k = -\xi_2 - 2D, \pi = 2\eta - 1 - \sqrt{\xi_1}s + \frac{D}{\sqrt{\xi_1}}, \tau = 1 - 2\sqrt{\xi_1}s + \frac{2D}{\sqrt{\xi_1}}.$$

From Eq.(19) we obtain energy equation as

$$2(n + 1)\sqrt{\xi_1} = -\xi_2 - 2D \quad (35)$$

Substituting  $\xi_1, \xi_2$  and  $D$  in Eq.(35) we obtain

$$\varepsilon = -\frac{B^2}{\lambda^2}(2A+1)^2 \left[ 2n+1 + \sqrt{(2\eta-1)^2 + \frac{V_0}{\lambda^2} + 2(\beta+1) - 4A^* - 4\eta(\eta-1)} \right]^{-2} \quad (36)$$

Using the same weight function defined in Eq.(32), we obtain

$$y_n(s) = B_n L_n^{\frac{2D}{\sqrt{\xi_1}}}(2\sqrt{\xi_1}s) \quad (37)$$

and also

$$\phi(s) = s^{2\eta-1+\frac{D}{\sqrt{\xi_1}}} e^{-\sqrt{\xi_1}s} \quad (38)$$

so total wave function becomes

$$\psi_n(s) = B_n s^{2\eta-1+\frac{D}{\sqrt{\xi_1}}} e^{-\sqrt{\xi_1}s} L_n^{\frac{2D}{\sqrt{\xi_1}}}(2\sqrt{\xi_1}s) \quad (39)$$

Eq.(34) and (35) are the general solutions of mass dependent Schrödinger equation which is given by Eq.(5) for the potential relation introduced in Eq.(7).

### 3.2 Solution of the Morse potential

In this case, we aim to obtain the solutions for the potential relation in Eq.(7) by reducing the mass dependent Schrödinger equation in Eq.(5) to a well-known Schrödinger equation with a Morse potential. The generalized Morse potential is

$$V(x) = V_1 e^{-2\alpha^*x} - V_2 e^{-\alpha^*x} \quad (40)$$

We write the SE for the potential in Eq. 40 by using a variable transformation,  $s = \sqrt{V_1} e^{-\alpha^*x}$  as

$$\frac{d^2\psi}{ds^2} + \frac{1}{s} \frac{d\psi}{ds} + \frac{1}{s^2} \left[ -\gamma^{*2} s^2 + \gamma^{*2} \frac{V_2}{\sqrt{V_1}} s - 4\varepsilon^{*2} \right] \psi = 0 \quad (41)$$



and

$$\varepsilon^{*2} = -\frac{mE^*}{2\hbar^2\alpha^{*2}} \quad (42)$$

and

$$\gamma^{*2} = \frac{2m}{\hbar^2\alpha^{*2}} \quad (43)$$

Comparing Eqs.(14) and (41), we define

$$\xi_1 = \gamma^{*2} \quad (44)$$

$$-\xi_2 = \frac{V_2}{\sqrt{V_1}}\gamma^{*2} \quad (45)$$

$$\xi_3 = -4\varepsilon^{*2} \quad (46)$$

$$D^2 = \xi_1[(2\eta - 1)^2 - \xi_3] \quad (47)$$

or

$$D = 2\gamma^*\varepsilon^* \quad (48)$$

For the values of  $\eta = \frac{1}{2}$ , mass dependent Schrödinger equation in Eq.(14) turns into Eq.(41) which is not mass dependent form for the Morse potential. From energy equation which is given by Eq.(29),

$$(2n + 1)\gamma^* = \frac{V_2}{\sqrt{V_1}}\gamma^{*2} + 4\gamma^*\varepsilon^* \quad (49)$$

is obtained. Thus, we solve

$$\varepsilon^* = \frac{1}{4} \left[ 2n + 1 - \frac{V_2}{\sqrt{V_1}}\gamma^* \right] \quad (50)$$

Taking  $\hbar = 1$ , we obtain the energy eigenvalues

$$E^* = -\frac{1}{4}\alpha^{*2} \left[ 2n + 1 - \frac{V_2}{\sqrt{V_1}}\gamma^* \right]^2 \quad (51)$$

From Eq.(34), we obtain

$$\psi_n(s) = B_n s^{-2\varepsilon^*} e^{-\gamma^* s} L_n^{-4\varepsilon^*} (2\gamma^* s) \quad (52)$$

or one can re-write the wave function from Eq.(50)

$$\psi_n(s) = B_n s^{-\frac{1}{2}\left(-2n+1-\frac{V_2}{\sqrt{V_1}}\gamma^*\right)} e^{-\gamma^* s} L_n^{\left(2n+1-\frac{V_2}{\sqrt{V_1}}\gamma^*\right)} (2\gamma^* s) \quad (53)$$

Eq.(53) which is the solutions of Eq.(41) is obtained by using Eq.(14). If we consider these solutions, solutions of Schrödinger equation including mass dependent parameters can be found.

This case is given in below.

## 4 Solutions within mass dependent parameters

If we recall Eqs.(11-13, 44-46),

$$\xi_1 = -\frac{\varepsilon}{\lambda^2} = \gamma^{*2} \quad (54)$$

$$\xi_2 = -\frac{B(2A+1)}{\lambda^2} = -\frac{V_2}{\sqrt{V_1}}\gamma^{*2} \quad (55)$$

$$-\xi_3 = \frac{V_0}{\lambda^2} + 2(\beta+1) - 4A^* + 1 = 4\varepsilon^{*2} \quad (56)$$

and

$$\varepsilon = -\lambda^2 \gamma^{*2} = -\frac{\sqrt{V_1}}{V_2} B(2A+1) \quad (57)$$

For the values of  $\varepsilon = -B^2$ , one can obtain  $B$  as

$$B = \frac{\sqrt{V_1}}{V_2}(2A + 1) \quad (58)$$

If we take  $\lambda = \gamma^* = \frac{1}{\alpha^*} = 1$ , we obtain  $B = 1$

$$\frac{V_2}{\sqrt{V_1}} = 2A + 1 \quad (59)$$

and from Eq. (52), the wave function becomes

$$\psi = B_n s^{-\sqrt{\frac{V_0}{\lambda^2} + 2(\beta+1) - 4A^* + 1}} e^{-\frac{1}{\lambda}\sqrt{-\varepsilon}s} L_n^{-2\sqrt{\frac{V_0}{\lambda^2} + 2(\beta+1) - 4A^* + 1}} \left( \frac{2}{\lambda}\sqrt{-\varepsilon}s \right) \quad (60)$$

From Eq.(52), relation of the wave function can be written as

$$\psi = B_n s^{-(n-A)} e^{-s} L_n^{-2(n-A)}(2s). \quad (61)$$

Using Eq.(36),  $\varepsilon = -B^2$ , and Eqs.(58, 59), we get

$$1 = (2A + 1)^2 \left[ 2n + 1 - 2\sqrt{\frac{V_0}{\lambda^2} + 2(\beta + 1) - 4A^* + 1} \right]^{-2}. \quad (62)$$

From Eq. (50), the energy is obtained. Substituting the expression of  $A^*$  in Eq.(9) and for the values of  $\lambda = 1$ ,  $V_0$

$$V_0 = (n - A)^2 + 4\alpha(\alpha + \beta + 1) + 2\beta + 1 \quad (63)$$

is obtained. The energy relation is obtained from Eqs.(42) and (59) can be given below

$$E^* = -(n - A)^2. \quad (64)$$

If this expression is used in Eq.(63),  $V_0$  has the following form

$$V_0 = -E^* + 4\alpha(\alpha + \beta + 1) + 2\beta + 1. \quad (65)$$

## 5 Conclusions

The effective mass Schrödinger equation is solved for a given potential. The Nikiforov-Uvarov method. is used to get energy eigenvalues and the corresponding wave functions in a general form by introducing a free parameter. By using this general form of the solutions of the effective mass Schrödinger equation, we have solved the effective mass Schrödinger equation for Morse potential transforming into a constant mass Schrödinger equation. We have shown that the effective mass Schrödinger equation can also be obtained starting from the constant mass case.

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