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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.

Keywords Position-dependent mass · Effective mass Schrödinger equation · Morse potential · Nikiforov-Uvarov method

1 Introduction

Quantum mechanical systems with spatially dependent effective mass (PDEM) has been extensively used in different branch of physics [1–5]. Applications have been increased in quantum mechanical problems and various approaches in the atomic, nuclear and other fields of physics in a PDEM background are also used [6, 7]. Several authors have investigated the exact solution of Schrödinger equation (SE) with position dependent mass using SUSY techniques [8–11]. Lie algebras for PDEM SE were used to obtain exact solutions of the effective mass wave equation [12–15]. Exact solutions of SE with different applications are given in [16–23].

Nikiforov-Uvarov (NU) approach has been introduced for solving SE, Klein-Gordon, Dirac and Salpeter equations [24–30]. In this work, NU method is adapted to the PDEM SE

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which is solved for a given potential. Energy eigenvalues and the corresponding wave functions are calculated. Then as an application the PDEM SE is solved for the Morse potential by transforming into a constant mass SE for a well known potential. Bagchi and collaborators work is followed for the shape of the position dependent mass function and potential parameters [31]. It is also shown that the solutions of the PDEM SE can be obtained by starting from the constant mass SE for the Morse potential.

The contents of the paper is as follows: in Sect. 2, we introduce PDEM approach and Nikiforov-Uvarov method. The next section involves applications to Morse potential. Solutions obtained with mass dependent parameters are given in Sect. 4. Results are discussed in Sect. 5.

2 Method

We write the one-dimensional effective mass Hamiltonian which is initially suggested by von Roos [5]

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

where V_{eff} has the form

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

with ambiguity parameters α, β and primes stand for the derivatives with respect to x. Dimensionless form $m(x)$ of the mass function is used and we have set $\hbar = 2m_0 = 1$ [26]. For constant m, problem reduces to the case of constant mass SE, so V_{eff} reduces to $V(x)$. Here, V_{eff} is the potential of the mass dependent equation, so depends on the mass terms and $V(x)$ is the potential that is chosen. Thus the SE takes the form

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

We apply the following transformation

$$\varphi = m^{\eta}(x)\,\psi(x) \tag{4}$$

Hence, the SE becomes

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

For the case of $\eta = 1/2$, this equation turns to (4) in [31]. Now we assume that

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

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

Substituting these relations into (5), we get

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

where

$$A^* = \alpha(\alpha + \beta + 1) + \beta + 1 \tag{9}$$

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

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

For simplicity, let us define

$$\xi_1 = -\frac{\varepsilon}{\lambda^2} \tag{11}$$

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

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

Thus, (10) has the form

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

Now, we apply NU method starting from its standard form. In this method, it is common to write the SE equation after an appropriate coordinate transformation $s = s(r)$ [24]:

$$\psi''_n(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0 \tag{15}$$

If we compare (14) and (15), it is obvious that we can obtain $\sigma, \tilde{\tau}, \tilde{\sigma}$ as

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

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 π and the parameter λ are defined as

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

and

$$\lambda = k + \pi' \tag{18}$$

To find the value of the expression under the square root, it must be square of a polynomial. Then, a new eigenvalue equation for the SE becomes

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

where

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

and it should have a negative derivative [24]. A family of particular solutions for a given λ 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

$$\psi(s) = \phi(s) y(s) \tag{21}$$

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

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

where $\rho(s)$ must satisfy the condition [24]

$$(\sigma\rho)' = \tau\rho \tag{23}$$

The other part is defined as a logarithmic derivative

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

3 Calculations

3.1 Solutions of (14) with the Nikiforov-Uvarov Method

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

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

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

$$\pi = 2\eta - 1 \tag{26}$$

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

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

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

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

Case I: $k = -\xi_2 + 2D$, $\pi = 1 - 2\eta - \sqrt{\xi_1}s - \frac{D}{\sqrt{\xi_1}}$, $\tau = 1 - 2\sqrt{\xi_1}s - \frac{2D}{\sqrt{\xi_1}}$.
From (19) we obtain energy equation as

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

Substituting ξ_1, ξ_2 and D in (29), we solve ε as

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

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

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

we compute $y_n(s)$ from (22) as

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

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

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

Thus, total wave function becomes

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

Case II: $k = -\xi_2 - 2D$, $\pi = 1 - 2\eta - \sqrt{\xi_1}s + \frac{D}{\sqrt{\xi_1}}$, $\tau = 1 - 2\sqrt{\xi_1}s + \frac{2D}{\sqrt{\xi_1}}$.
From (19) we obtain energy equation as

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

Substituting ξ_1, ξ_2 and D in (35), we obtain

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

Using the same weight function defined in (32), y_n can be introduced as

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

and also ϕ is given as:

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

So total wave function becomes

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

Equations (34) and (39) are the general solutions of mass dependent Schrödinger equation which is given by (5) for the potential relation introduced in (7).

3.2 Solution of the Morse Potential

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

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

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

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

and

$$\varepsilon^{*2} = -\frac{mE^*}{2\hbar^2\alpha^{*2}} \tag{42}$$

and

$$\gamma^{*2} = \frac{2m}{\hbar^2\alpha^{*2}} \tag{43}$$

Comparing (14) and (41), we define

$$\xi_1 = \gamma^{*2} \tag{44}$$

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

$$\xi_3 = -4\varepsilon^{*2} \tag{46}$$

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

or

$$D = 2\gamma^*\varepsilon^* \tag{48}$$

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

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

is obtained. Thus, we solve

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

Setting $\hbar = 2m = 1$ in (42) and (43), we can obtain the energy eigenvalues

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

From (34), we obtain

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

or one can re-write the wave function from (52)

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

Equation (53) which is the solutions of (41) is obtained by using (14). Here, (51) and (53) are free of mass dependent parameters. Solutions of Schrödinger equation including mass dependent parameters can be found. This case is given in below.

4 Solutions within Mass Dependent Parameters

One can also follow a reverse process for obtaining the solutions in this problem. Mass dependent parameters will be used for the exact solutions of PDEM SE by some transformations. If we recall (11)–(13), (44)–(46),

$$\xi_1 = -\frac{\varepsilon}{\lambda^2} = \gamma^{*2} \tag{54}$$

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

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

and

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

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

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

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

$$\frac{V_2}{\sqrt{V_1}} = 2A+1 \tag{59}$$

Using (52), the wave function becomes

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

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

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

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

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

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

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

is obtained. The energy relation is obtained from (50) and (59) can be given below

$$E^* = -(n - A)^2 \tag{64}$$

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

$$V_0 = -E^* + 4\alpha(\alpha + \beta + 1) + 2\beta + 1 \tag{65}$$

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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