A New Vision on Schrödinger Equation Using Position Dependent Mass Concerning Modified Hylleraas-Hulthén Potential Expanded by Nikiforov-Uvarov Method

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Abstract

Schrödinger equation is developed starting with position-dependent mass considering the quantum interacting potentials in quantum mechanics, that such called a modified Hylleraas-Hulthén potential where its developed using the Nikiforov-Uvarov approach. The wave functions are investigated and the energy eigenvalues and the related eigenfunctions are also determined

Keywords: Position-dependent mass Schrödinger equation, Nikiforov-Uvarov method, modified Hylleraas-Hulthén potential.

1. Introduction

The Schrödinger equation with a position-dependent mass (PDM) is a variation of the standard Schrödinger equation in quantum physics. Although the Schrödinger equation is believed to have a constant mass for every particle, but in some physical systems, particularly in condensed and nanoscale physics, a particle's mass can alter its position. The main interesting idea is to provide a clear impression and description about Schrödinger equation that depends on altering mass position.

Numerous studies on quantum systems with PDM have been achieved [1-3]. Very valuable models in many practical fields, including current physics, are the Schrödinger equations with a PDM. PDM have spread over various applications in condensed physics include the study of semiconductor electronic characteristics [4-5], quantum wells and quantum dots [6–8], graded alloys and semiconductor heterostructures [9], quantum liquids [10], etc.

Otherwise, several analytical methods, including the factorization approach [11], Darboux transformation [12], Nikiforov-Uvarov method (NU) [13], point canonical transformation [14], and supersymmetry, shape invariance [15–16], have been used to solve the Schrodinger equation using several potential models, such as Kratzer potential, Poschl-Teller potential, Morse potential, Coulomb potential, and Hulthén potential. [17–18] .

But the most exceptional thing in this study that we indicate a new interaction between two quantum potentials, which is the Modified Hylleraas Potential [19–20] and the Hulthén Potential [21–23]; to deal with more complex systems with three particles. The first potential is applied to simulate the interaction of three charged particles in a quantum system that concerned mostly in the molecular physics. The original Hylleraas potential, is that express the electron-electron interaction in helium atoms But to deal with more complex systems with three particles, the Modified Hylleraas Potential provides more words. It is fortunately applied to the study triatomic molecules or systems involving the interaction of three charged particles, like electrons or nuclei, while the second potential is applied to express the interaction of two particles in quantum physics. This potential fortunately, in atomic and molecular physics, is applied to simulate the interaction of a charged particle

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(such as an electron) with a nucleus. In quantum physics, this potential is frequently applied to examine confined states and scattering processes. This interesting model is helpful for many analytical and computational applications because it is spread to cover some important aspects of the interaction among particles with charge. That is concerned as an essential step in demonstrating the position-dependent mass Schrödinger equation (PDMSE) for such systems to determining the potential energy function, that acts the forces between these particles.

We seek to investigate the Schrödinger equation with PDM operating the Nikiforov-Uvarov (NU) method concerning modified Hylleraas-Hulthén potential determining the energy level and associated wave function. Now, This paper constructed as follows: Section 2 provides the Schrödinger equation with PDM. The review of the NU method is the focus of Section 3. Section 4 provides the analytical solution to the PDM Schrödinger equation for modified Hylleraas- Hulthén potential using NU method. Lastly, Section 5, the conclusion and final statement.

Position-dependent mass Schrödinger equation

The general PDM Hamiltonian proposed by Von Roos with $\hbar = 2m_0 = 1$ is

$$H_{eff} = -\frac{1}{2} \left(M^{\alpha}(x) \frac{d}{dx} M^{\beta}(x) \frac{d}{dx} M^{\gamma}(x) + M^{\gamma}(x) \frac{d}{dx} M^{\beta}(x) \frac{d}{dx} M^{\alpha}(x) \right) + V_{eff}(x)$$
 (1)

The dimensionless form of the function $m(x) = m_0 M(x)$ is M(x), and its parameters are $\alpha + \beta + \gamma = -1$. Von Roos settled the limitation $\alpha = \gamma = 0$ and $\beta = -1$, which are introduced as the ambiguity parameters.

Concerning the above parameters in equation (1), the one-dimensional effective mass Hamiltonian is as follows:

$$H_{eff} = -\frac{d}{dx} \left(\frac{1}{m(x)}\right) \frac{d}{dx} + V_{eff}(x) \tag{2}$$

Then the PDM Schrödinger equation assumes the form:
$$\left[-\frac{1}{m(x)} \frac{d^2}{dx^2} + \frac{m'(x)}{m^2(x)} \frac{d}{dx} + V_{eff}(x) - E \right] \varphi(x) = 0$$
 Where the V_{eff}(x) is

$$V_{eff}(x) = V(x) + \frac{1}{2}(\beta + 1)\frac{m''(x)}{m^2(x)} - \left[\alpha(\alpha + \beta + 1) + (\beta + 1)\right]\frac{m'^2(x)}{m^3(x)}$$
(4)

 α , β are ambiguity parameters.

After employing the transformation [24] $\varphi(x) = m^{\upsilon}(x)\psi(x)$ and using equation (4) into (3) we get

$$\left[-\frac{d^2}{dx^2} - (2v - 1)\frac{m'(x)}{m(x)}\frac{d}{dx} + \left(\frac{1}{2}(\beta + 1) - v\right)\frac{m''(x)}{m(x)} - \left(v(v - 2) + \alpha(\alpha + \beta + 1) + (\beta + 1)\right)\frac{m'^2(x)}{m^2(x)} + m(x)(V(x) - E)\right]\psi = 0$$
(5)

The PDM Schrödinger equation is identified as the preceding equation.

In the next section, we're going to provide a detailed overview about Nikiforov-Uvarov (NU) method.

3. NU Method

The rules of the (NU) approach [25] are the managing of specific orthogonal functions to solve second-order differential equations of the hypergeometric type. The Schrödinger or PDM Schrödinger equation can be settled systematically to provide the precise or specific solutions for a given potential by reducing them to a generalized equation of hypergeometric type with the suitable coordinate transformation. The following displays the main equation that is strongly allied to the methodology.

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \tag{6}$$

International Journal of Multiphysics

Volume 18, No. 2, 2024

ISSN: 1750-9548

Where $\tilde{\tau}(s)$ is a polynomial of first degree, $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of degree at most two, $\psi(s)$ is a hypergeometric type function.

The common form of Schrodinger equation is expressed for any potential as

$$\left[\frac{d^2}{ds^2} + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \frac{d}{ds} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{s^2 (1 - s)^2}\right] \psi = 0$$
 (7)

Equation (6) can be solved specifically by multiplying two different components of the wave function, which are as follows, once the variables have been separated:

$$\psi(s) = \varphi(s)y(s) \tag{8}$$

Where $\varphi(s)$ is defined as a logarithmic derivative:

$$\frac{\varphi'(s)}{\varphi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{9}$$

 $\pi(s)$ is a polynomial with one degree or less.

If we consider the preceding transformation equation (6) as a hypergeometric equation:

$$\sigma(s)y_n''(s) + \tau(s)y_n'(s) + \lambda y_n(s) = 0$$
 (10)

Where

$$\tau(s) = 2\pi(s) + \tilde{\tau}(s) \tag{11}$$

Suppose $\tau'(s) < 0$, this condition assist to produce physical solutions.

Rodrigues relation gives the solution of the hypergeometric-type function $y_n(s)$ of (8) as:

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)]$$
 (12)

Where n is a fixed integer, $\rho(s)$ is the weight function, and B_n is the normalization constant.

The following differential equation is determined by the weight function.

$$\frac{d}{ds}[\sigma(s)\rho(s)] = \tau(s)\rho(s) \tag{13}$$

Or

$$\frac{\rho'(s)}{\rho(s)} = \frac{\tau(s) - \sigma'(s)}{\sigma(s)} \tag{14}$$

Then $\pi(s)$ is set as:

$$\pi(s) = \frac{\sigma' - \tilde{\tau}(s)}{2} \pm \sqrt{(\frac{\sigma' - \tilde{\tau}(s)}{2})^2 - \tilde{\sigma}(s) + k\sigma(s)}$$
 (15)

And

$$k = \lambda - \pi'(s) \tag{16}$$

Therefore, for the computation of $\pi(x)$, the most crucial step is to find k by setting the discriminant of the square root in (15) to zero. Additionally, the equation for the eigenvalue provided in (16) well be declared as:

$$\lambda = \lambda_n = -n \, \tau' - \frac{n(n-1)}{2} \sigma''(s) \,, (n = 0, 1, 2, ...)$$
 (17)

Here, the prime represents the first-degree differentials.

4. Results and Discussion

The modified Hylleraas potential is given by

$$V(x) = \frac{V_0}{b} \left(\frac{a - e^{-2\lambda x}}{1 - e^{-2\lambda x}} \right)$$
 (18)

Where λ is the inverse of the potential's range and V_0 , the potential well's depths, are the Hylleraas parameters a and b.

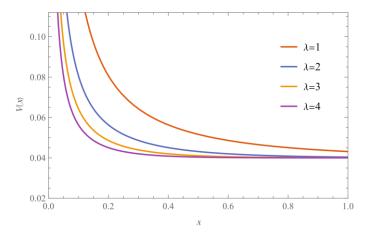


Fig. 1. Modified Hylleraas potential with $V_0=1$, a=2 and b=50.

$$V(x) = -V_1 \frac{e^{-2\lambda x}}{1 - e^{-2\lambda x}}$$
 (19)

Where V_1 , is the potential depth.

One of the recognizable short-range potentials is the Hulthén potential, which displays an exponential drop for high values of x and a Coulomb potential behavior for small values of x. In its most essential form, the Hulthén potential is expressed as:

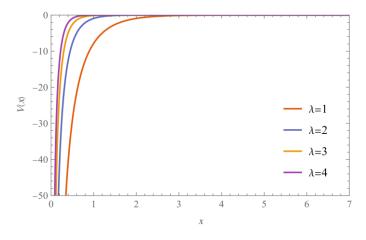


Fig. 2. Hulthén potential with $V_1 = 50$.

Our newly interesting interacting potential, which is provided by combining equations, is called the Modified Hylleraas- Hulthén Potential (MHHP). (18) as well as (19):

$$V(x) = \frac{V_0}{b} \left(\frac{a - e^{-2\lambda x}}{1 - e^{-2\lambda x}} \right) - V_1 \frac{e^{-2\lambda x}}{1 - e^{-2\lambda x}}$$
 (20)

And this the (MHHP) plotting

Obtaining the mass altering

$$m(x) = \frac{m_0}{(1 - e^{-2\lambda x})} \tag{21}$$

Figure (3) displays the mass function's behavior.

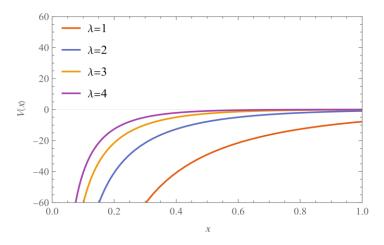


Fig. 3. MHHP with $V_0 = 1$, $V_1 = 50$.

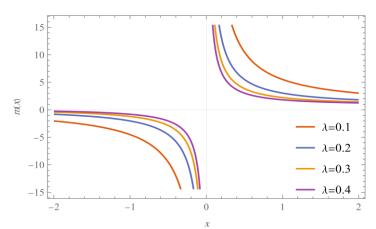


Fig. 4. Variation of the PDM function of different value of λ and $m_0=1.$

The derivatives:

$$m'(x) = \frac{-2\lambda e^{-2\lambda x}}{(1 - e^{-2\lambda x})^2}$$
 (22)

And

$$m''(x) = 2\lambda^{2} \left[\frac{4e^{-4\lambda x}}{(1 - e^{-2\lambda x})^{3}} + \frac{2e^{-2\lambda x}}{(1 - e^{-2\lambda x})^{2}} \right]$$
 (23)

After that, we get these parameters

$$\frac{m'(x)}{m(x)} = \frac{-2\lambda e^{-2\lambda x}}{(1 - e^{-2\lambda x})}$$
(24)

And

$$\frac{m''(x)}{m(x)} = 2\lambda^2 \left[\frac{4e^{-4\lambda x}}{(1 - e^{-2\lambda x})^2} + \frac{2e^{-2\lambda x}}{(1 - e^{-2\lambda x})} \right]$$
 (25)

Demonstrating equations (20), (21), (24), and (25) into equation (5)

$$\begin{split} \left[-\frac{d^2}{dx^2} - (2\upsilon - 1) \frac{-2\lambda e^{-2\lambda x}}{(1 - e^{-2\lambda x})} \frac{d}{dx} + \left(\frac{1}{2} (\beta + 1) - \upsilon \right) 2\lambda^2 \left[\frac{4e^{-4\lambda x}}{(1 - e^{-2\lambda x})^2} + \frac{2e^{-2\lambda x}}{(1 - e^{-2\lambda x})} \right] \\ - \left(\upsilon (\upsilon - 2) + \alpha (\alpha + \beta + 1) + (\beta + 1) \right) \frac{4\lambda^2 e^{-4\lambda x}}{(1 - e^{-2\lambda x})^2} \\ + \frac{1}{(1 - e^{-2\lambda x})} \left(\frac{V_0}{b} \left(\frac{a - e^{-2\lambda x}}{1 - e^{-2\lambda x}} \right) - V_1 \frac{e^{-2\lambda x}}{1 - e^{-2\lambda x}} - E \right) \right] \psi = 0 \end{split}$$
 (26)

Now, changing variable

$$s = \frac{1}{(1 - e^{-2\lambda x})}, (0 \le s \le 1)$$
 (27)

Equation (26) is transport to the Nikiforov-Uvarov equation by changing this variable. After this change, (24) and (25) becomes

$$\frac{m'(x)}{m(x)} = 2\lambda(1-s) \tag{28}$$

And

$$\frac{m''(x)}{m(x)} = 4\lambda^2 (1 - s)(1 - 2s)$$
 (29)

After using the transformation in (26), it becomes

$$\begin{split} &\left[\frac{d^2}{dx^2} + \frac{2\upsilon - (2\upsilon + 1)s}{s(1-s)}\frac{d}{dx} + \left[-4\lambda^2\left(\frac{1}{2}(\beta+1) - \upsilon\right)(1-s)(1-2s) + 4\lambda^2\left(\upsilon(\upsilon-2) + \alpha(\alpha+\beta+1) + (\beta+1)\right)(1-s)^2 - \frac{1}{(1-e^{-2\lambda x})}\left(\frac{aV_0 - V_0e^{-2\lambda x}}{b - be^{-2\lambda x}} - V_1\frac{e^{-2\lambda x}}{1-e^{-2\lambda x}} - E\right)\right]\psi = 0 \end{split} \tag{30}$$

In order to simplify (30), we set

$$C_1 = (\eta(\eta - 2) + \alpha(\alpha + \beta + 1) + (\beta + 1)) \tag{31}$$

$$C_2 = \left(\frac{1}{2}(\beta + 1) - \upsilon\right) \tag{32}$$

$$C_3 = \frac{1}{2} - \upsilon \tag{33}$$

Thus

$$\begin{split} \left[\frac{d^2}{dx^2} + \frac{2\upsilon - (2\upsilon + 1)s}{s(1-s)} \frac{d}{dx} \\ & + \left[4\lambda^2 C_1 (1-s)^2 - 4\lambda^2 C_2 (1-s)(1-2s) - \frac{1}{(1-e^{-2\lambda x})} \left(\frac{V_0}{b} \left(\frac{a-e^{-2\lambda x}}{1-e^{-2\lambda x}} \right) \right. \right. \end{aligned} \tag{34}$$

$$\left. - V_1 \frac{e^{-2\lambda x}}{1-e^{-2\lambda x}} - E \right] \right] \psi = 0 \end{split}$$

Expanding (34)

$$\begin{split} \frac{d^2 \psi}{ds^2} + \frac{2\upsilon - (2\upsilon + 1)s}{s(1-s)} \, \frac{d\psi}{ds} \\ + \left[C_1 - 2C_1 s + C_1 s^2 - C_2 + 3C_2 s - 2C_2 s^2 \right. \\ \left. + \left(-\frac{V_0}{b} \frac{a - e^{-2\lambda x}}{4\lambda^2 (1 - e^{-2\lambda x})^2} + V_1 \frac{e^{-2\lambda x}}{4\lambda^2 (1 - e^{-2\lambda x})^2} + \frac{E}{4\lambda^2 (1 - e^{-2\lambda x})} \right) \right] \psi = 0 \end{split}$$
 (35)

International Journal of Multiphysics

Volume 18, No. 2, 2024

ISSN: 1750-9548

Then

$$\begin{split} \frac{d^2 \psi}{ds^2} + \frac{2 \upsilon - (2 \upsilon + 1) s}{s (1 - s)} \, \frac{d \psi}{ds} \\ + \left[C_1 - 2 C_1 s + C_1 s^2 - C_2 + 3 C_2 s - 2 C_2 s^2 \right. \\ \left. + \left(- \frac{V_0}{b} \frac{a - e^{-2 \lambda x}}{4 \lambda^2 (1 - e^{-2 \lambda x})^2} + V_1 \frac{e^{-2 \lambda x}}{4 \lambda^2 (1 - e^{-2 \lambda x})^2} + \frac{E}{4 \lambda^2 (1 - e^{-2 \lambda x})} \right) \right] \psi = 0 \end{split}$$
 (36)

Rearranging the terms enclosed in brackets Equation (36) can be transport to the generalized hypergeometric-type equation, which is the parametric generalization of the NU method.

$$\frac{d^{2}\psi}{ds^{2}} + \frac{2\upsilon - (2\upsilon + 1)s}{s(1 - s)} \frac{d\psi}{ds} + \frac{1}{s^{2}(1 - s)^{2}} \left[\left(C_{1} - 2C_{2} - \frac{V_{0}(a - 1)}{4b\lambda^{2}} + \frac{V_{1}}{4\lambda^{2}} \right) s^{2} + \left(-2C_{1} + 3C_{2} - \frac{V_{0}(a - 1)}{4b\lambda^{2}} + \frac{V_{1}}{4\lambda^{2}} + \frac{E}{4\lambda^{2}} \right) s + (C_{1} - C_{2}) \right] \psi(x) = 0$$
(37)

Where

$$\begin{split} \gamma_1 &= -C_1 + 2C_2 + \frac{V_0(a-1)}{4b\lambda^2} - \frac{V_1}{4\lambda^2} \\ \gamma_2 &= -2C_1 + 3C_2 - \frac{V_0(a-1)}{4b\lambda^2} + \frac{V_1}{4\lambda^2} + \frac{E}{4\lambda^2} \\ \gamma_3 &= -C_1 + C_2 \end{split} \tag{38}$$

Now equation (37) displayed as

$$\frac{d^2\psi}{ds^2} + \frac{2\upsilon - (2\upsilon + 1)s}{s(1-s)} \frac{d\psi}{ds} + \frac{1}{s^2(1-s)^2} [-\gamma_1 s^2 + \gamma_2 s - \gamma_3] \psi(x) = 0 \tag{39}$$

After comparing (39) with (6), we have

$$\begin{split} \tilde{\tau}(s) &= 2\upsilon - (2\upsilon + 1)s \\ \sigma(s) &= s(1-s) \\ \tilde{\sigma}(s) &= -\gamma_1 s^2 + \gamma_2 s - \gamma_3 \end{split} \tag{40}$$

Using these polynomials in equation (15), we have

$$\pi(s) = \left(\frac{1}{2} - \upsilon\right) (1 - s) \pm \begin{cases} \left(\sqrt{\mu} - \eta\right)s + \eta \; ; k = \gamma_2 - 2\gamma_3 + 2\eta\sqrt{\mu} \\ \left(\sqrt{\mu} + \eta\right)s - \eta \; ; \; k = \gamma_2 - 2\gamma_3 - 2\eta\sqrt{\mu} \end{cases}$$
(41)

Thus

$$\mu = \sqrt{\frac{V_1}{4\lambda^2} + \frac{E}{4\lambda^2}}$$

$$\eta^2 = \left(\frac{\beta}{2}\right)^2 - \left(\alpha + \frac{\beta + 1}{2}\right)^2$$
(42)

Now by choosing this value of k

$$k = \gamma_2 - 2\gamma_3 - 2\eta\sqrt{\mu} \tag{43}$$

With

$$\pi(s) = \left(\frac{1}{2} - \upsilon\right)(1 - s) - \left(\sqrt{\mu} + \eta\right)s + \eta \tag{44}$$

Now, using equation (11) to calculate the polynomial $\tau(s)$

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$$\tau(s) = 2[\left(\frac{1}{2} - \upsilon\right)(1 - s) - \left(\sqrt{\mu} + \eta\right)s + \eta] + 2\upsilon - (2\upsilon + 1)s \tag{45}$$

We have

$$\tau(s) = 1 - 2s - 2((\sqrt{\mu} + \eta)s - \eta) \tag{46}$$

The derivative is expressed as:

$$\tau'(s) = -2\left(1 + \sqrt{\mu} + \eta\right) \tag{47}$$

From (16) and (17)

$$\lambda = \lambda_n = -2n(-1 - (\sqrt{\mu} + \eta)) + n(n-1) \tag{48}$$

We have

$$\lambda = \gamma_1 - (\sqrt{\mu} + \eta)^2 - (\sqrt{\mu} + \eta) + \upsilon^2 - \frac{1}{4}$$
 (49)

Comparing (48) and (49)

$$\left(\sqrt{\mu} + \eta\right) = -\left(n + \frac{1}{2}\right) \pm \upsilon \sqrt{\frac{\gamma_1}{\upsilon^2} + 1} \tag{50}$$

The energy levels

$$E_{n} = -4\lambda^{2} \left[(2n+1) - \sqrt{\frac{V_{0}(a-1) - bV_{1}}{4b\lambda^{2}} - \alpha(\alpha+\beta+1)} - \sqrt{\left(\frac{\beta}{2}\right)^{2} - \left(\alpha + \frac{\beta+1}{2}\right)^{2}} \right]^{2} - V_{1} \quad (0 \le n < \infty)$$
(51)

Now, we can provide the numerical analysis of E_n, for different values of the parameters a and b.

Table.1. Numerical outcomes of energy spectra for a=20, b=0.5, α =0, β =-1, V0=50, and V1=100

	CJ 1	, , , , ,
	λ	En
n		
0	1	-1816.14718
1	2	-1151.47186
2	3	-337.97403
3	4	-191.65369

And it's displayed as:

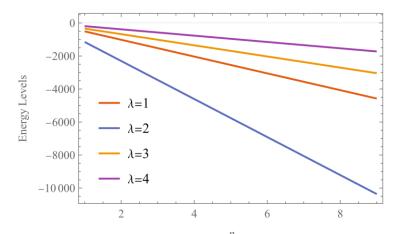


Fig. 5. MHH energy levels for $a = 20, b = 0.5, \alpha = 0, \beta = -1, V_0 = 50, \text{ and } V_1 = 100$

Table.2. Numerical outcomes of energy spectra for a=9, b=0.1, α =0, β =-1, V0=50, and V1=100

n	λ	E _n
0	1	-3876.10004
1	2	-2851.00040
2	3	-1356.70108
3	4	-209.20208

And its displayed as:

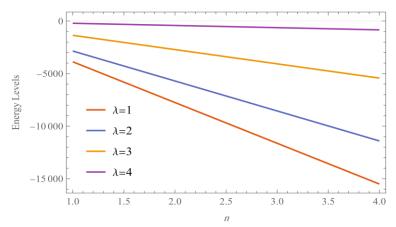


Fig. 6. MHH energy levels for a = 9, b = 0.1, $\alpha = 0$, $\beta = -1$, $V_0 = 50$, and $V_1 = 100$ From the above analysis, we can notice that as the values of the parameters are low, the energy states decrease.

Now the weight function obtaining using (11), (14), and (46).

$$\rho(s) = s^{2\eta} (1 - s)^{2\sqrt{\mu}} \tag{52}$$

Using equation (52), the solution of y defined from (12) can expressed as:

$$y_n(s) = C_n s^{-2\eta} (1-s)^{-2\sqrt{\mu}} \frac{d^n}{ds^n} [s^{n+2\eta} (1-s)^{n+2\sqrt{\mu}}]$$
 (53)

From (9), (40), (43) and (54), we have

$$\varphi(s) = s^{\left(\frac{1}{2} - \upsilon\right) + \eta} (1 - s)^{\sqrt{\mu}} \tag{54}$$

And now from these properties of Jacobi polynomial's [3]

$$P_n^{(\eta,\sqrt{\mu})}(x) = \frac{(-1)^n (1-x)^{-\eta} (1+x)^{-\sqrt{\mu}}}{2^n n!} \frac{d^n}{dx^n} [(1-x)^{n+\eta} (1+x)^{n+\sqrt{\mu}}] \tag{55}$$

And

$$P_n^{(2\eta,2\sqrt{\mu})}(1-2s) = \frac{(-2)^n(s)^{-2\eta}(1-s)^{-2\sqrt{\mu}}}{2^n n!} \frac{d^n}{dx^n} [s^{n+2\eta}(1-s)^{n+2\sqrt{\mu}}]$$
 Where the Jacobi polynomial is $P_n^{(a,b)}(x)$, (a > -1, b > -1). Thus we have:

$$y_n(s)=P_n^{(2\eta,2\sqrt{\mu})}(1-2s) \eqno(57)$$
 Lastly, we highly represent the wave functions $\psi_n(s),$ using (8), (12), (53), and (54)

$$\psi_n(s) = N_n s^{\left(\frac{1}{2} - \upsilon\right) + \eta} (1 - s)^{\sqrt{\mu}} P_n^{(2\eta, 2\sqrt{\mu})} (1 - 2s) \tag{58}$$

Where N_n is the normalization constant. We can find it by this normalizing condition.

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1 = \int_{0}^{1} |\psi_n(s)|^2 ds$$
 (59)

5. Conclusion

The PDM Schrodinger equation in this research, is managed with MHHP involving NU approach to demonstrate the valuable system's energy and wave function, successfully. The effects of the potential and the parameters on the system's energy spectra are demonstrated and displayed explicitly by a numerical and graphic analysis of the energy spectra. This integrated model proves precisely the wave function, energy spectra, and the eigen values concerning triatoms potentials, altering position mass dependent merging between quantum and molecular principle. These system-specific ideas would offer a far more comprehensive and examine to understand molecular interactions.

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