Approximate Analytical Solutions of the Perturbed Yukawa Potential with Centrifugal Barrier

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By using the generalized parametric Nikiforov–Uvarov (NU) method, we have obtained the approximate analytical solutions of the radial Schrödinger equation for a perturbed Yukawa potential. The energy eigenvalues and corresponding eigenfunctions are calculated in closed forms. Some numerical results are presented and compared with the standard Yukawa potential. Further, we found the energy levels of the familiar Mie-type potential when the screening parameter of the perturbed Yukawa potential goes to zero, and finally, standard Yukawa and Coulomb potentials are discussed.

Key words: Schrödinger Equation; Perturbed Yukawa Potential; Mie-Type Potential; Nikiforov–Uvarov Method.

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1. Introduction

Solutions of fundamental dynamical equations are of great interest in many fields of physics and chemistry. In this regards, the exact solutions of the radial Schrödinger equation for a hydrogen atom (Coulombic) and a harmonic oscillator represent two typical examples in quantum mechanics [1–4]. The radial Schrödinger equation has been solved with different potentials and methods [5–10].

The perturbed Yukawa potential is given by

\[ V(r) = -V_0 \frac{e^{-ar}}{r} + V_1 \frac{e^{-2ar}}{r^2}, \quad V_1 \ll V_0, \quad (1) \]

where \( V_0 = \alpha Z \) with the fine-structure constant \( \alpha = (137.0337)^{-1} \) and the atomic number \( Z \); \( a \) is the screening parameter. When \( V_1 \) is zero, the potential (1) reduces to the standard Yukawa potential [11] which is often used to compute bound-state normalizations and energy levels of neutral atoms [12–14]. This potential has been solved by the shifted large-\( N \) [15], perturbative [16–18], supersymmetry quantum mechanic [19], asymptotic iteration [20], quasi-linearization [21], and Nikiforov–Uvarov [22–25] methods.

This work is arranged as follows: in Section 2, the parametric generalization NU method with all the necessary formulae used in the calculations is briefly introduced. In Section 3, we solve the radial Schrödinger equation for the perturbed Yukawa potential and give energy spectra and corresponding wave functions. Some numerical results and discussions are given in this section, too. Finally, the relevant conclusion and some remarks are given in Section 4.

2. Parametric NU Method

This powerful mathematical tool solves second-order differential equations. Let us consider the following differential equation [26–29]:

\[ \psi''_{\nu} (s) + \frac{\tau(s)}{\sigma(s)} \psi'_{\nu} (s) + \frac{\sigma(s)}{\sigma^2(s)} \psi_{\nu} (s) = 0, \quad (2) \]

where \( \sigma(s) \) and \( \sigma(s) \) are polynomials, at most of second degree, and \( \tau(s) \) is a first-degree polynomial. The application of the NU method can be made simpler and direct without need to check the validity of solution. We present a shortcut for the method. So, at first we write the general form of the Schrödinger-like equation (2) in a more general form as
\[
\psi_n'(s) + \left( \frac{c_1 - c_5 s}{s(1-c_3 s)} \right) \psi_n'(s) + \left( -p_1 s^2 + p_{1s} - p_0 \right) s^2(1-c_3 s)^2 \psi_n(s) = 0, \tag{3}
\]
satisfying the wave functions
\[
\psi_n(s) = \varphi(s) y_n(s). \tag{4}
\]
Comparing (3) with its counterpart (2), we obtain the following identifications:
\[
\tilde{\tau}(s) = c_1 - c_2 s, \quad \sigma(s) = s(1-c_3 s), \quad \tilde{\sigma}(s) = -p_2 s^2 + p_{1s} - p_0. \tag{5}
\]
(i) For the given root \(k_1\) and the function \(\pi_1(s)\), we get
\[
k = -(c_7 + 2c_3 c_8) - 2\sqrt{c_8 c_9}, \quad \pi(s) = c_4 + \sqrt{c_8} - \left( \sqrt{c_9} + \sqrt{c_8 c_9} - c_5 \right) s.
\]
Now we follow the NU method [27–29] to obtain the energy equation
\[
nc_2 - (2n+1)c_5 + (2n+1)\left( \sqrt{c_9} + c_13 \sqrt{c_8} \right) + n(n-1)c_3 + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0 \tag{6}
\]
and the wave functions
\[
\rho(s) = s^{10}(1-c_3 s)^{c_13}, \quad \varphi(s) = s^{12}(1-c_3 s)^{c_13}, \quad c_{12} > 0, \quad c_{13} > 0, \quad y_n(s) = P_n^{(c_0,c_11)}(1-2c_3 s), \quad c_{10} > -1, \quad c_{11} > -1, \tag{7}
\]
\[
\psi_{nl}(s) = N_{nl}s^{c_12}(1-c_3 s)^{c_13} P_n^{(c_0,c_11)}(1-2c_3 s).
\]
\(P_n^{(\mu,v)}(x)\), \(\mu > -1, \nu > -1\), and \(x \in [-1,1]\) are Jacobi polynomials with the constants being
\[
c_4 = \frac{1}{2} (1-c_1), \quad c_5 = \frac{1}{2} (c_2 - 2c_3), \quad c_6 = c_2^2 + p_2, \quad c_7 = 2c_4 c_5 - p_1, \quad c_8 = c_2^2 + p_0, \quad c_9 = c_3(c_7 + c_3 c_8) + c_6, \quad c_{10} = 2\sqrt{c_8} > -1, \quad c_{11} = \frac{2}{c_3} \sqrt{c_9} > -1, \quad c_3 \neq 0, \tag{8}
\]
\[
c_{12} = c_4 + \sqrt{c_8} > 0, \quad c_{13} = -c_4 + \frac{1}{c_3} \sqrt{c_9 - c_5} > 0, \quad c_3 \neq 0,
\]
where \(c_{12} > 0, c_{13} > 0, \) and \(s \in [0, 1/c_3], c_3 \neq 0.\)

In the rather more special case of \(c_3 = 0\), the wave function (7) becomes
\[
\lim_{c_3 \to 0} P_n^{(c_0,c_11)}(1-2c_3 s) = L_n^{c_10}(2\sqrt{c_9} s), \quad \lim_{c_3 \to 0} (1-c_3 s)^{c_13} = e^{-(\sqrt{c_9} - c_3 s)}, \tag{9}
\]
\[
\psi(s) = N_s s^{c_12} e^{-(\sqrt{c_9} - c_3 s)} L_n^{c_10}(2\sqrt{c_9} s).
\]
(ii) For the given root \(k_2\) and the function \(\pi_2(s)\), we have
\[
k = -(c_7 + 2c_3 c_8) + 2\sqrt{c_8 c_9}, \quad \pi(s) = c_4 - \sqrt{c_8} - \left( \sqrt{c_9} - c_3 \sqrt{c_8} - c_5 \right) s.
\]
following the NU method [29] to obtain the energy equation
\[
nc_2 - (2n+1)c_5 + (2n+1)\left( \sqrt{c_9} - c_3 \sqrt{c_8} \right) + n(n-1)c_3 + c_7 + 2c_3 c_8 - 2\sqrt{c_8 c_9} = 0 \tag{10}
\]
and the wave functions
\[
\rho(s) = s^{10}(1-c_3 s)^{c_11}, \quad \varphi(s) = s^{12}(1-c_3 s)^{c_13}, \quad c_{12} > 0, \quad c_{13} > 0, \quad y_n(s) = P_n^{(c_0,c_11)}(1-2c_3 s), \quad c_{10} > -1, c_{11} > -1, \tag{11}
\]
\[
\psi_{nl}(s) = N_{nl}s^{c_12}(1-c_3 s)^{c_13} P_n^{(c_0,c_11)}(1-2c_3 s),
\]
where
\[
\tilde{c}_{10} = -2\sqrt{c_8}, \quad \tilde{c}_{11} = \frac{2}{c_3} \sqrt{c_9}, \quad \tilde{c}_9 \neq 0, \quad \tilde{c}_{12} = c_4 - \sqrt{c_8} > 0, \quad \tilde{c}_{13} = -c_4 + \frac{1}{c_3} \left( \sqrt{c_9} - c_5 \right) > 0, \quad c_3 \neq 0. \tag{12}
\]

3. Solution of the Radial Schrödinger Equation with the Perturbed Yukawa Potential

To study any quantum physical system characterized by the empirical potential given in (1), we solve the original Schrödinger equation which is given in well-known textbooks [1, 2]:
\[
\left( \frac{\mu^2}{2} + V(r) \right) \psi(r, \theta, \varphi) = E \psi(r, \theta, \varphi), \tag{13}
\]
where \(\mu\) is the reduced mass, and the potential \(V(r)\) is taken as the perturbed Yukawa potential in (1). Using the separation method with the wave function \(\psi(r, \theta, \varphi) = R_l(r)Y_{lm}(\theta, \varphi)\), we obtain the following radial Schrödinger equation:
\[
\left[ \frac{d^2}{dr^2} + 2\mu \left( E + V_0 \frac{e^{-ar}}{r} - V_1 \frac{e^{-2ar}}{r^2} \right) - \frac{l(l+1)}{r^2} \right] R_n(r) = 0.
\]  

(14)

Since the radial Schrödinger equation with the perturbed Yukawa potential has no exact solution, we use an approximation for the centrifugal term in the form

\[
\frac{1}{r^2} \approx 4a^2 \frac{e^{-2ar}}{(1 - e^{-2ar})^2},
\]

or equivalently

\[
\frac{1}{r} \approx 2a - \frac{e^{-ar}}{1 - e^{-2ar}},
\]

which is valid for \( ar \ll 1 \) [30]. Therefore, the perturbed Yukawa potential in \( (1) \) reduces to \([31, 32]\)

\[
V(r) = -2aV_0 \frac{e^{-2ar}}{(1 - e^{-2ar})} + 4a^2V_1 \frac{e^{-4ar}}{(1 - e^{-2ar})^2}.
\]  

(17)

To see the accuracy of our approximation, we plotted the perturbed Yukawa potential \( (1) \) and its approximation \( (17) \) with parameters \( V_0 = \sqrt{2} \) and \( a = 0.10 \) [20] in Figure 1. Substituting \( (15) \) and \( (16) \) into \( (14) \), one obtains

\[
\frac{d^2 R_n(s)}{ds^2} + \frac{1}{s(1-s)} \frac{d R_n(s)}{ds} + \frac{1}{s^2(1-s)^2} \left[ -\varepsilon + 1 - \mu V_0 \right] R_n(s) = \frac{(1-s)}{a} R_n(s).
\]  

(19)

Comparing \( (19) \) and \( (3) \), we can easily obtain the coefficients \( c_i \) \( (i = 1, 2, 3) \) and analytical expressions \( p_j \) \( (j = 0, 1, 2) \) as follows:

\[
c_1 = 1, \quad p_1 = \frac{\mu V_0}{a} + \frac{\varepsilon}{4a^2} + 2\mu V_1, \\
c_2 = 1, \quad p_1 = 2 \frac{\varepsilon}{4a^2} + \frac{\mu V_0}{a} - l(l+1), \\
c_3 = 1, \quad p_0 = \frac{\varepsilon}{4a^2}.
\]  

(20)

The values of coefficients \( c_i \) \( (i = 4, 5, \ldots, 13) \) can be found from \( (8) \) and are displayed in Table 1. By

![Fig. 1 (colour online). Perturbed Yukawa potential (red line) and its approximation in (17) (blue dash dot line) with \( V_0 = \sqrt{2} \) and \( a = 0.10 \).](image)

Fig. 1 (colour online). Perturbed Yukawa potential (red line) and its approximation in (17) (blue dash dot line) with \( V_0 = \sqrt{2} \) and \( a = 0.10 \).
using (6), we obtain the energy eigenvalues of the perturbed Yukawa potential as

\[
E_{\text{el}} = -\frac{a^2}{2\mu} \left( \frac{\mu V_0}{a} \right)^2 \left( \frac{l+\frac{1}{2}}{2} \right)^2 - \left( n + \frac{1}{2} \right)^2 \left( l + \frac{1}{2} \right) + (2n+1) \left( 2 \mu V_1 \right)^2 \left( n + \frac{1}{2} \right)^2 \left( l + \frac{1}{2} \right)^2 - 2 (n+1) \left( \frac{l+\frac{1}{2}}{2} \right)^2 + 2 \mu V_1 \right)^{-2} \left( n + \frac{1}{2} \right) \left( l + \frac{1}{2} \right)^{2} + 2 \mu V_1 \right)^{-2}.
\]

(21)

Some numerical results are given in Tables 2–4. In Table 2, we used the parameters $\hbar = \mu = 1$, $V_0 = \sqrt{\alpha}$, $a = (0.002V_0, 0.005V_0, 0.010V_0, 0.020V_0, 0.025V_0, 0.050V_0)$ [20], $V_1 = \pm 0.05$ and obtained the energy eigenvalues of the perturbed Yukawa potential for various states and compared them with the approximate and numerical energy eigenvalues of the standard Yukawa potential [33]. In Tables 3 and 4, we show the numerical results with parameter set $\hbar = 2\mu = 1$, $a = 0.2 \text{ fm}^{-1}$ for the heavy and light atoms $V_0 = \alpha Z = 4$ to $V_0 = \alpha Z = 24$ and compared them with the standard Yukawa potential. As one can see from Tables 1–3, we must note that our solution is only correct for the lowest $l$-states as we approximated the centrifugal term.

When the screening parameter $a$ approaches zero, $V_0 = 2D \alpha r_e$ and $V_1 = D \alpha r_e^2$, the potential (1) reduces to the Mie-type potential [4]. Thus, in this limit the energy eigenvalues of (19) become the energy levels of the Mie-type interaction, i.e.

\[
E_{\text{mie}} = -2\mu r_e^2 D_e \left( n + \frac{1}{2} \right) + \left( \frac{l+\frac{1}{2}}{2} \right)^2 + 2 \mu r_e^2 D_e \right)^{-2}.
\]

(22)

Table 2. Energy eigenvalues (in fm$^{-1}$) of the perturbed Yukawa and standard Yukawa potentials in units $\hbar = \mu = 1$. We set $V_0 = \sqrt{\alpha}$ for comparison with other methods.

<table>
<thead>
<tr>
<th>State</th>
<th>$a$</th>
<th>perturbed Yuk. $V_1 = 0.05$</th>
<th>perturbed Yuk. $V_1 = -0.05$</th>
<th>standard Yuk. $V_1 = 0$</th>
<th>standard Yuk. (Numerical [33])</th>
</tr>
</thead>
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<td>-0.83534</td>
<td>-1.26566</td>
<td>-0.99600</td>
<td>-0.99600</td>
</tr>
<tr>
<td></td>
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<td>-0.99000</td>
</tr>
<tr>
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<td>-0.98010</td>
</tr>
<tr>
<td></td>
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<td>-0.96040</td>
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<tr>
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<tr>
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</tr>
<tr>
<td>2s</td>
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</tr>
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</table>
Table 3. Same as in Table 2, but $\hbar = 2\mu = 1$, $a = 0.2$ fm$^{-1}$, and $n = 0$.

<table>
<thead>
<tr>
<th>$V_0$</th>
<th>$l$</th>
<th>$E_{\text{perturbed Yuk}}$ at $V_1 = 0.05$</th>
<th>$E_{\text{perturbed Yuk}}$ at $V_1 = -0.05$</th>
<th>$E_{\text{standard Yuk}}$ at $V_1 = 0$ (Analytical [33])</th>
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<tbody>
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<td>1</td>
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</tbody>
</table>

which is identical to (30) of [34, 35]. Also, when $V_1 = 0$, potential (1) reduces to the standard Yukawa potential [22, 23] and its energy levels can be obtained from (21) as

$$E_{\text{nlYukawa}} = \frac{\alpha^2}{2\mu} \left( \frac{\mu V_0}{\alpha} - (n + l + 1)^2 \right)$$

under the physical condition $n + l + 1 \leq \sqrt{\mu V_0/\alpha}$ [22]. When the screening parameter $\alpha$ approaches zero, the standard Yukawa potential reduces to a Coulomb potential. Thus, in this limit the energy eigenvalues of (23) become the energy levels of the pure Coulomb interaction, i.e.

$$E_{\text{nlCoulomb}} = -\frac{1}{2} \frac{V_0^2}{n'^2},$$

where $n' = n + l + 1$ [1, 2, 35].

To find corresponding wave functions, referring to Table 1 and (7), we find the radial wave functions as

$$R_{nl}(s) = N_{nl} s \sqrt{\frac{a}{4\pi \alpha}} \left( 1 - s \right)^{\frac{1}{2}} \left( 1 + \frac{l + \frac{1}{2}}{2\mu V_1} \right)^{\frac{1}{2}}$$

or, by substituting $s = e^{-2\alpha r}$,

$$R_{nl}(r) = N_{nl} e^{-\sqrt{\alpha r}} \left( 1 - e^{-2\alpha r} \right)^{\frac{1}{2}} \left( 1 + \frac{l + \frac{1}{2}}{2\mu V_1} \right)^{\frac{1}{2}}$$

where $N_{nl}$ is a normalization constant. As mentioned, when the screening parameter $\alpha$ approaches zero, $V_0 = 2D_s r_c$ and $V_1 = D_e r_c^2$, the potential (1) reduces to the Mie-type potential [4]. In this limit, we have $c_5 = 0$ and the wave function can be obtained from (9). Therefore the radial wave functions of Mie-type potential become [35].

Table 4. Same as in Table 3, but $n > 0$.

<table>
<thead>
<tr>
<th>$V_0$</th>
<th>$n$</th>
<th>$l$</th>
<th>$E_{\text{perturbed Yuk}}$ at $V_1 = 0.05$</th>
<th>$E_{\text{perturbed Yuk}}$ at $V_1 = -0.05$</th>
<th>$E_{\text{standard Yuk}}$ at $V_1 = 0$ (Analytical [33])</th>
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<tbody>
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See the next page for the remaining content.
\[ R_{\text{nl}} = N_{\text{nl}} e^{-\sqrt{V(r)}} \left( 1 - e^{-\sqrt{V(r)}} \right)^{-1} \left( 2\sqrt{V(r)} \right) \]

Also, when the screening parameter \( a \) approaches zero and \( V_1 = 0 \), our problem reduces to the Coulomb one and the radial wave functions become \([1, 2, 35]\)

\[ R_{\text{nlCoulomb}} = N_{\text{nl}} e^{-\sqrt{V(r)}} \left( 1 - e^{-\sqrt{V(r)}} \right)^{-1} \left( 2\sqrt{V(r)} \right) \]

4. Conclusion and Remarks

In this article, we have obtained the bound state solutions of the Schrödinger equation for a perturbed Yukawa potential by using the parametric generalization of the Nikiforov–Uvarov method. The energy eigenvalues and corresponding eigenfunctions are obtained by this method. Some numerical results are given in Table 2 and compared with the standard Yukawa potential. It is found that when the screening parameter \( a \) goes to zero, the energy levels approach to the familiar Mie-type potential energy levels. The aim of solving the perturbed Yukawa potential returns to the following reasons: First, in the low screening region where the screening parameter \( a \) is small (i.e., \( a \ll 1 \)), the potential reduces to the Killingbeck potential \([36, 37]\), i.e., \( V(r) = a^2 + br - c/r \), where \( a, b, \) and \( c \) are potential constants that can be obtained after making expansion to the perturbed Yukawa potential. Second, it can also be reduced into the Cornell potential \([38, 39]\), i.e., \( V(r) = br - c/r \). These two potentials are usually used in the study of mesons and baryons.

Third, when the screening parameter approaches to zero, the perturbed Yukawa potential turns to become the Mie-type potential. Finally, we discussed standard Yukawa and pure Coulomb potential.

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