Research Article

Bound State Solutions of Three-Dimensional Klein-Gordon Equation for Two Model Potentials by NU Method

N. Tazimi [ID] and A. Ghasempour [ID]

Department of Physics, University of Kashan, Kashan, Iran

Correspondence should be addressed to N. Tazimi; nt_physics@yahoo.com

In this study, we investigate the relativistic Klein-Gordon equation analytically for the Deng-Fan potential and Hulthen plus Eckart potential under the equal vector and scalar potential conditions. Accordingly, we obtain the energy eigenvalues of the molecular systems in different states as well as the normalized wave function in terms of the generalized Laguerre polynomials function through the NU method, which is an effective method for the exact solution of second-order linear differential equations.

1. Introduction

The exact solution is of paramount importance in quantum mechanics as it carries essential information on the quantum systems under investigation. It is possible only for quantum systems such as H_2 and harmonic oscillator. As for the majority of quantum systems, the approximation method needs to be used. In most quantum systems, for the analytical solution, methods such as the Nikiforov-Uvarov method [1], quantization rules [2], ansatz method [3], supersymmetry (SUSY) method [4], and series expansion [5] have been used for any arbitrary l state.

Recently, the bound state of the Schrödinger equation has been solved by the Deng-Fan potential [6], modified Morse potential [7], and Eckart potential [8] by approximation to the centrifugal term, and the wave function and energy level for bound states in any arbitrary l state have been identified. The bound state solutions of the Klein-Gordon equation with the Deng-Fan molecular potential are solved by Dong [9]. Wei et al. investigated the relativistic scattering states of the Hulthen potential by taking the same approximation [10]. Wei and Dong examined the approximate solution of the bound state of the Dirac equation with the second Pöschl-Teller potential under spin symmetry conditions and with scalar and vector modified potentials under pseudospin symmetry conditions [11, 12]. They also solved the Dirac equation with the scalar and vector Manning-Rosen potentials under pseudospin symmetry conditions by using the function analysis method and algebraic formalism [13].

In our previous works, we solved the Schrödinger equation for different potentials for few-quark systems [14–17]. However, in the present work, we make use of the NU method to solve the Klein-Gordon equation for a diatomic molecule analytically. The NU method has recently been exploited in a variety of physical fields, including the Schrödinger equation with a spherically harmonic oscillatory ring-shaped potential [18] or the second Pöschl-Teller-like potential by the Nikiforov-Uvarov method [19].

In this paper, first we describe the Nikiforov-Uvarov method. In Review of Nikiforov-Uvarov (NU) Method, we consider the Deng-Fan potential and calculate the energy eigenvalue for different diatomic molecules. Next, we solve the Klein-Gordon equation analytically for the Eckart plus Hulthen potential through the NU method and obtain the energy eigenvalue. And finally, we present the results, discussion, and conclusion.

2. Review of Nikiforov-Uvarov (NU) Method

The Schrödinger equation can be converted into a second-order differential equation as follows:

$$\sigma''(s) + \frac{d^2\psi(s)}{ds^2} + \sigma(s)\tilde{\tau}(s)\frac{d\psi(s)}{ds} + \tilde{\sigma}(s)\psi(s) = 0, \qquad (1)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ denote polynomials at most of the second degree and $\tilde{\tau}(s)$ is a first-degree polynomial. We use the following form to find the solution:

$$\Psi(s) = \psi(s)\varphi(s). \qquad (2)$$

By introducing Equation (3) into Equation (2), we arrive at

$$\sigma(s)\frac{d^2\varphi(s)}{ds^2} + \tau(s)\frac{d\varphi(s)}{ds} + \lambda\varphi(s)0, \qquad (3)$$

where $\varphi(s)$ in terms of the Rodriguez formula appears as

$$\varphi_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}[\sigma^n(s)\rho(s)]. \qquad (4)$$

The weight function $\rho(s)$ holds in the following formula:

$$\frac{d\psi(s)}{ds} + \frac{\sigma(s)}{\rho(s)}\frac{d\rho(s)}{ds} = \tau(s). \qquad (5)$$

The other solution factor is defined as

$$\pi(s) = \frac{1}{2}\left[\sigma'(s) - \tilde{\tau}(s)\right] \pm \left\{\left[\sigma'(s) - \tilde{\tau}(s)\right]^2 - \tilde{\sigma}(s) + k\sigma(s)\right\}^{1/2}. \qquad (6)$$

In this method, the polynomial $\pi(s)$ and parameter k are defined as

$$k = \lambda - \pi'(s), \qquad (7)$$

where $\psi(s)$ is defined as

$$\frac{1}{\psi(s)}\frac{d\psi(s)}{ds} = \frac{\pi(s)}{\psi(s)}. \qquad (8)$$

By substituting k into Equation (7):

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \qquad (9)$$

and λ is defined as:

$$\lambda = \lambda_n = -n\tau' - \frac{\left[n(n-1)\sigma''\right]}{2}, \qquad n = 0, 1, 2, \cdots. \qquad (10)$$

The general form of the Schrödinger equation including any potential is

$$\frac{d^2\psi(s)}{ds^2} + \left(\frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)}\right)\frac{d\psi(s)}{ds} + \left(\frac{-As^2 + Bs - C}{s^2(1 - \alpha_3 s)^2}\right)\psi(s) = 0. \qquad (11)$$

Comparing Equation (12) with Equation (2), we get the parameters

$$\begin{aligned}
\tilde{\tau}(s) &= \alpha_1 - \alpha_2, \\
\sigma(s) &= s(1 - \alpha_3 s), \\
\tilde{\sigma}(s) &= -As^2 + Bs - C.
\end{aligned} \qquad (12)$$

Based on the equations, the constant parameters are defined as

$$\begin{aligned}
\alpha_4 &= \frac{1}{2}(1 - \alpha_1), \\
\alpha_5 &= \frac{1}{2}(\alpha_2 - 2\alpha_3), \\
\alpha_6 &= \alpha_5^2 + A, \\
\alpha_7 &= 2\alpha_4\alpha_5 - B, \\
\alpha_8 &= \alpha_4^2 + C, \\
\alpha_9 &= \alpha_3\alpha_7 + \alpha_3^2\alpha_8 + \alpha_6, \\
\alpha_{10} &= \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8}, \\
\alpha_{11} &= \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}), \\
\alpha_{12} &= \alpha_4 + \sqrt{\alpha_8}, \\
\alpha_{13} &= \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}).
\end{aligned} \qquad (13)$$

The energy equation is obtained from

$$\begin{aligned}
\alpha_2 n - (2n+1)\alpha_5 + (2n+1)(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) + n(n-1)\alpha_3 \\
+ \alpha_7 + 2\alpha_3\alpha_8 + 2\sqrt{\alpha_8\alpha_9} = 0.
\end{aligned} \qquad (14)$$

Now we consider the eigenfunctions of the problem with any potential. We obtain the second part of the solution from Equation (4).

$$\phi_n(s) = P_n^{(\alpha_{10}-1,(\alpha_{11}/\alpha_3)-\alpha_{10}-1)}(1 - 2\alpha_3 s). \qquad (15)$$

From the explicit form of the weight function obtained from Equation (5), we arrive at

$$\rho(s) = s^{\alpha_{10}-1}\left(1 - \alpha_3 s^{(\alpha_{11}/\alpha_3)-\alpha_{10}-1}\right). \qquad (16)$$

$P_n^{(\alpha,\beta)}(1 - 2\alpha_3 s)$ is the Jacobi polynomial. From Equation (6), we arrive at

$$\psi(s) = s^{\alpha_{12}}(1 - \alpha_3 s)^{-\alpha_{12}-(\alpha_{13}/\alpha_3)}. \qquad (17)$$

Then the general solution $\Psi(s)\psi(s)\phi(s)$ becomes

$$\psi(s) = s^{\alpha_{12}}(1 - \alpha_3 s)^{-\alpha_{12} - (\alpha_{13}/\alpha_3)} \times P_n^{(\alpha_{10}-1, (\alpha_{11}/\alpha_3) - \alpha_{10} - 1)}(1 - 2\alpha_3 s).$$

(18)

3. Solving the Klein-Gordon Equation for the Ground State

The potential that is selected for molecular spectroscopy and molecular dynamics is of paramount importance. The Deng-Fan oscillator potential [20] is a simple potential model for diatomic molecules. It has the correct physical boundary conditions at $r = 0$ and ∞. It is defined by

$$V(r) = D\left(1 - \frac{b}{e^{\alpha r} - 1}\right)^2, \quad b = e^{\alpha r_e} - 1, \quad r \in (0, \infty), \quad (19)$$

where D stands for the dissociation energy, r_e for the equilibrium bond length, and α for the potential range. The shifted Deng-Fan potential is of the following form (Figure 1)

$$V(r) = D\left(1 - \frac{b}{e^{\alpha r} - 1}\right)^2 - D = D\left(\frac{-2b}{e^{\alpha r} - 1} + \frac{b^2}{(e^{\alpha r} - 1)^2}\right).$$

(20)

The radial part of the Klein-Gordon equation for a particle with a mass m and potential $V(r)$ is

$$\frac{d^2\varphi(r)}{dr^2} + \left\{\frac{1}{(\hbar c)^2}\left[(E^2 - m^2) - 2(E + m)V(r)\right] - \frac{l(l+1)}{r^2}\right\}\varphi(r) = 0.$$

(21)

Because of the term $1/r^2$ in Equation (21), it cannot be analytically solved except for $l = 0$. Therefore, a suitable approximation to the centrifugal term is required, as used in [9, 21, 22]:

$$\frac{1}{r^2} = \alpha^2\left(d_0 + \frac{1}{e^{\alpha r} - 1} + \frac{1}{(e^{\alpha r} - 1)^2}\right),$$

(22)

in which $\alpha r \ll 1$ and $d_0 = 1/12$. As illustrated in Figure 2, this approximation is very close to the term $1/r^2$. By introducing the potential and the approximation $1/r^2$ and $\hbar c = 1$, Equation (21) becomes

$$\frac{d^2\varphi(r)}{dr^2} + \left\{E^2 - m^2 + \frac{4bD(E+m)}{e^{\alpha r} - 1} - \frac{2b^2 D(E+m)}{(e^{\alpha r} - 1)^2}\right.$$
$$\left. - l(l+1)\alpha^2 d_0 - \frac{l(l+1)\alpha^2}{e^{\alpha r} - 1} - \frac{l(l+1)\alpha^2}{(e^{\alpha r} - 1)^2}\right\}\varphi(r) = 0.$$

(23)

By using the variable change $s = e^{-\alpha r}$ which maps the half-line $(0, \infty)$ into the interval $(0, 1)$, Equation (23) becomes

$$\frac{d^2\varphi(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{d\varphi}{ds} + \left\{\frac{E^2 - m^2}{\alpha^2 s^2} + \frac{4bD(E+m)}{\alpha^2 s(1-s)}\right.$$
$$\left. - \frac{2b^2 D(E+m)}{\alpha^2(1-s)^2} - \frac{l(l+1)d_0}{s^2} - \frac{l(l+1)}{s(1-s)} - \frac{l(l+1)}{(1-s)^2}\right\}\varphi(s) = 0.$$

(24)

By comparing Equations (11) and (24), the following coefficients are obtained:

$$\gamma^2 = -\left(\frac{E^2 - m^2}{\alpha^2}\right),$$
$$A = \gamma^2 + \beta^2 + \nu^2 + l(l+1)d_0,$$
$$\beta^2 = \frac{4bD(E+m)}{\alpha^2},$$
$$B = 2\gamma^2 + \beta^2 + (2d_0 - 1)l(l+1)$$
$$\nu^2 = \frac{2b^2 D(E+m)}{\alpha^2},$$
$$C = \gamma^2 + l(l+1)d_0.$$

(25)

By combining Equations (23) and (11), the following quantities are obtained:

$$\alpha_1 = \alpha_2 = \alpha_3 = 1,$$
$$\alpha_4 = 0,$$
$$\alpha_5 = -\frac{1}{2},$$
$$\alpha_6 = \frac{1}{4} + A,$$
$$\alpha_7 = -B,$$
$$\alpha_8 = C,$$
$$\alpha_9 = A - B + C + \frac{1}{4},$$
$$\alpha_{10} = 1 + 2\sqrt{C},$$
$$\alpha_{11} = 2 + 2\left(\sqrt{A - B + C + \frac{1}{4}} + \sqrt{C}\right),$$
$$\alpha_{12} = \sqrt{C},$$
$$\alpha_{13} = -\frac{1}{2} - \left(\sqrt{A - B + C + \frac{1}{4}} + \sqrt{C}\right).$$
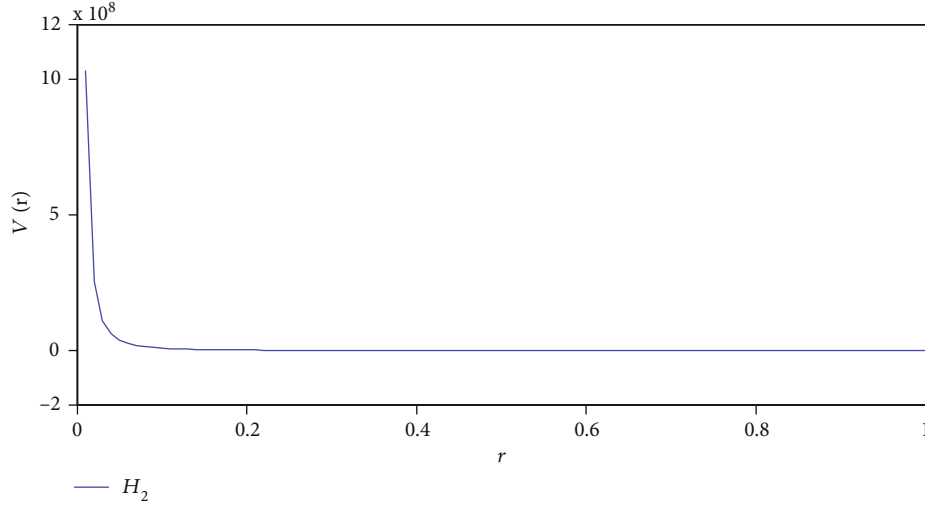
(26)

FIGURE 1: The Deng-Fan potential (eV) in terms of $r(A^0)$ for H_2 diatomic molecule.
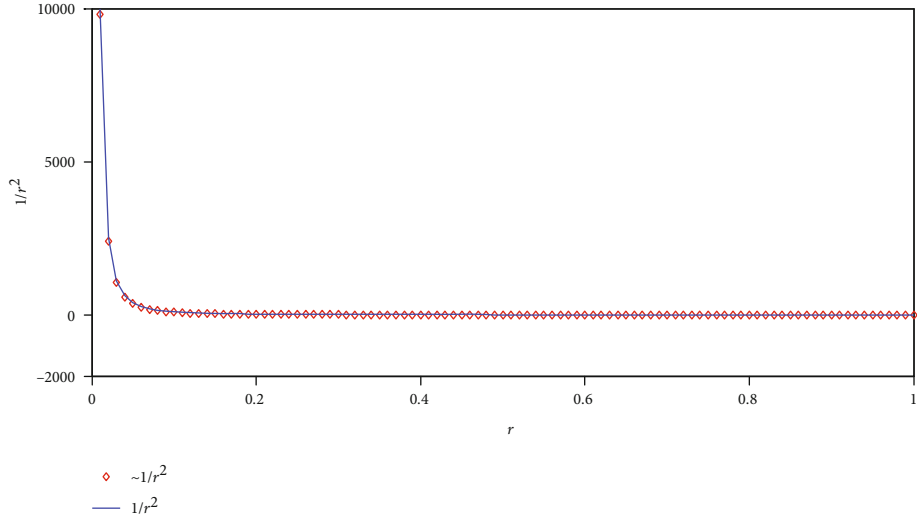

FIGURE 2: Comparision between $1/r^2$ of the Deng-Fan potential and the approximation scheme as function of r for H_2 diatomic molecule.

Finally, we find the energy eigenvalue as

$$E^2 - m^2 = -\alpha^2 \left(\frac{-n^2 + \beta^2 - l(l+1) - (2n+1)\delta'}{2(n+\delta')} \right)^2 + l(l+1)d_0\alpha^2, \tag{27}$$

in which

$$\delta' = \frac{1}{2}\left(1 + \sqrt{4v^2 + (2l+1)^2}\right). \tag{28}$$

In Table 1, we present potential parameters adopted from [23–25]. Furthermore, by the following data, we obtain the energy eigenvalue for diatomic molecules mentioned in Table 1.

TABLE 1: The potential model parameters for some diatomic molecules [18–20].

Molecule	$\mu(amu)$	$\alpha\left(A^{0^{-1}}\right)$	$r_e\left(A^0\right)$	$D\left(cm^{-1}\right)$
H_2	0.50391	1.9426	0.7416	38,266
LiH	0.8801221	1.1280	1.5956	20,287
CO	6.8606719	2.2994	1.1283	90,540
HCl	0.9801045	1.8677	1.2746	37,255

$$\hbar c = 1973.27 evA^0, \quad 1amu = 931.494028 Mev/C^2$$

$$d_0 = \frac{1}{12}, \quad V(r) = \frac{V(r)}{2},$$

$$E - m = E_{nl}, \quad E + m = \frac{2\mu}{\hbar^2}. \tag{29}$$

In Table 2, we calculate energy levels for different n and l states and compare them with other findings in [23, 24, 26, 27]. The radial wave function is of the following form:

$$
\begin{aligned}
R_{nl}(r) &= N_{nl} e^{-\sqrt{C}\alpha r} (1 - e^{-\alpha r})^{\delta_l} P_n^{(2\sqrt{C}, 2\delta_l - 1)} (1 - 2e^{-\alpha r}) \\
&= N_{nl} \frac{\left(2\sqrt{C} + 1\right)_n}{n!} e^{-\sqrt{C}\alpha r} (1 - e^{-\alpha r})^{\delta_l} {}_2F_1\left(-n, n \right. \\
&\quad \left. + 2\sqrt{C} + 2\delta_l ; 1 + 2\sqrt{C} ; e^{-\alpha r}\right),
\end{aligned} \quad (30)
$$

where

$$
\begin{aligned}
{}_2F_1 & \left(-n, n + \nu + \mu + 1 ; \nu + 1 ; \frac{1-x}{2}\right) \\
&= \frac{n!}{(\nu + 1)_n} P_n^{(\nu, \mu)}(x)(\nu + 1)_n = \frac{\Gamma(n + \nu + 1)}{\Gamma(\nu + 1)}.
\end{aligned} \quad (31)
$$

N_{nl} is the normalization constant. $P_n^{(\nu, \mu)}$ denotes the Jacobi polynomial and ${}_2F_1$ stands for the hypergeometric function. The N_{nl} constant is defined as

$$
\int_0^\infty |R_{nl}(r)|^2 dr = \int_0^1 |R_{nl}(s)|^2 \frac{ds}{\alpha s} = 1,
$$

$$
\begin{aligned}
|N_{nl}|^2 & \int_0^1 s^{2\sqrt{C}-1} (1-s)^{2\delta_l} \left[{}_2F_1\left(-n, n + 2\sqrt{C} + 2\delta_l ; 2\sqrt{C} + 1 ; s\right)\right]^2 ds \\
&= \alpha \left(\frac{n! \Gamma\left(2\sqrt{C} + 1\right)}{\Gamma\left(2\sqrt{C} + n + 1\right)}\right)^2.
\end{aligned} \quad (32)
$$

By using the following formula [28, 29]:

$$
\begin{aligned}
& \int_0^1 s^{2a-1} (1-s)^{2(b+1)} \left[{}_2F_1(-n, n + 2(a+b+1) ; 2a+1 ; s)\right]^2 ds \\
&= \frac{(n+b+1)n! \Gamma(n+2b+1)\Gamma(2a)\Gamma(2a+1)}{(n+a+b+1)\Gamma(n+2a+1)\Gamma(n+2(a+b+1))} \\
&\qquad\qquad\qquad\qquad a > -1/2, \quad b > -3/2,
\end{aligned} \quad (33)
$$

the normalization constant is obtained as

$$
N_{nl} = \sqrt{\frac{2\sqrt{C}\alpha n! \left(n + \sqrt{C} + \delta_l\right) \Gamma\left(n + 2\left(\sqrt{C} + \delta_l\right)\right)}{(n+\delta_l)\Gamma\left(n + 2\sqrt{C} + 1\right)\Gamma(n + 2\delta_l)}}, \quad (34)
$$

and for the ground state $n = 0$

$$
N_{0l} = \sqrt{\frac{\alpha\left(\sqrt{C} + \delta_l\right)}{\delta_l B\left(2\sqrt{C}, 2\delta_l\right)}},
$$

TABLE 2: The energy levels for a few diatomic molecules obtained from the sDF and Morse oscillator potentials.

n	l	$-E_{nl}$(eV) NU	$-E_{nl}$(eV) AP21, 22	$-E_{nl}$(eV) 19, 20
H_2				
0	0	4.39444	4.39444	4.47601
	5	4.17644	4.18054	4.25880
	10	3.62165	3.63782	3.72194
5	0	1.75835	1.75835	2.22052
	5	1.61731	1.62548	2.04355
	10	1.26034	1.29257	1.60391
7	0	1.07756	1.07756	1.53744
	5	0.96174	0.97232	1.37565
	10	0.66976	0.71172	0.97581
LiH				
0	0	2.41195	2.41195	2.42886
	5	2.38348	2.38458	2.40133
	10	2.30815	2.31229	2.32884
5	0	1.51628	1.51628	1.64771
	5	1.49278	1.49429	1.62377
	10	1.43062	1.43627	1.56074
7	0	1.22340	1.22340	1.37756
	5	1.20173	1.20344	1.35505
	10	1.14444	1.15083	1.29580
CO				
0	0	11.08068	11.08068	11.0915
	5	11.07247	11.07354	11.0844
	10	11.05057	11.05449	11.0653
5	0	9.68809	9.68809	9.79518
	5	9.68017	9.68130	9.78833
	10	9.65905	9.66321	9.77009
7	0	9.15911	9.15911	9.29918
	5	9.15131	9.15247	9.29246
	10	9.13050	9.13476	9.27455
HCl				
0	0	4.41705	4041705	4.43556
	5	4.37403	4.37843	4.39682
	10	4.25973	4.27591	4.29408
5	0	2.66574	2.66574	2.80506
	5	2.62859	2.63411	2.77209
	10	2.52989	2.55027	2.68471
7	0	2.09652	2.09652	2.25701
	5	2.06161	2.06768	2.22634
	10	1.96888	1.99127	2.14511

$$
B\left(2\sqrt{C}, 2\delta_l\right) = \frac{\Gamma\left(2\sqrt{C} + 1\right)\Gamma(2\delta_l)}{2\sqrt{C}\Gamma\left(2\sqrt{C} + 2\delta_l\right)}. \quad (35)
$$

We plot wavefunction of the Deng-Fan potential (eV) as a function of $r(A^0)$ for the H_2 diatomic molecule in $n = l = 0$ in Figure 3.
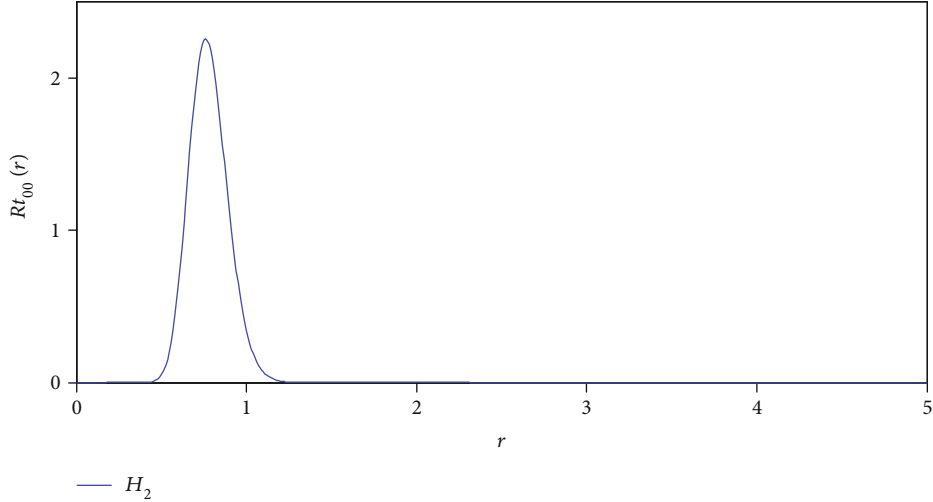
FIGURE 3: Wave function (eV) in terms of $r(A^0)$ of Deng-Fan potential for H_2 diatomic molecule ($n = l = 0$) in atomic units $y = \mu = 1$.

4. Eckart plus Hulthen Potential

The Eckart plus Hulthen potential has been used for the analytical solution of the Schrödinger equation. This potential as a diatomic molecular potential model has been utilized in applied physics and chemical physics. The NU method has been exploited to solve the Schrödinger equation for the Eckart plus Hulthen potential [30]. However, in the present work, we make use of the NU method to solve the Klein-Gordon equation for the Eckart plus Hulthen potential. The Eckart plus Hulthen potential runs as shown in Figure 4:

$$V(r) = \operatorname{cosec} \mathrm{h}^2(ar) + \coth(ar) + \frac{V_0}{(1 - e^{-2\alpha r})} - \frac{V_1}{(1 - e^{-2\alpha r})^2},$$

(36)

where V_0 and V_1 stand for the depths of potential well and α for the inverse of the potential range. The hyperbolic functions are defined as

$$\sinh(\alpha r) = \frac{e^{\alpha r} - e^{-\alpha r}}{2},$$

$$\cosh(\alpha r) = \frac{e^{\alpha r} + e^{-\alpha r}}{2},$$

(37)

$$\tanh(\alpha r) = \frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}.$$

In this way, the potential is obtained as

$$V(r) = \frac{4e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} + \frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \frac{V_0}{1 - e^{-2\alpha r}} - \frac{V_1}{(1 - e^{-2\alpha r})^2}.$$

(38)

The radial Klein-Gordon equation by using the Eckart plus Hulthen potential in $l = 0$ is of the following form:

$$\frac{d^2\varphi(r)}{dr^2} + \left\{ E^2 - m^2 - \frac{4(E + m)e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} - (E + m)\frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right.$$
$$\left. - (E + m)\frac{V_0}{1 - e^{-2\alpha r}} + (E + m)\frac{V_1}{(1 - e^{-2\alpha r})^2} \right\}\varphi(r) = 0.$$

(39)

With the variable change $s = e^{-2\alpha r}$, Equation (40) is transformed to

$$\frac{d^2\varphi(s)}{ds^2} + \frac{(1 - s)}{s(1 - s)}\frac{d\varphi}{ds} + \frac{1}{s^2(1 - s)^2}\left\{ \frac{E^2 - m^2(1 - s^2)}{4\alpha^2} \right.$$
$$- \frac{(E + m)s}{\alpha^2} - \frac{(E + m)}{4\alpha^2}(1 + s)(1 - s) - \frac{(E + m)V_0(1 - s)}{4\alpha^2}$$
$$\left. + \frac{(E + m)V_1}{4\alpha^2} \right\}\varphi(s) = 0.$$

(40)

With a simple comparison, the following quantities are obtained:

$$\gamma^2 = -\left(\frac{E^2 - m^2}{4\alpha^2}\right),$$

$$A = \gamma^2 + \beta^2,$$

$$\beta^2 = -\frac{(E + m)}{4\alpha^2},$$
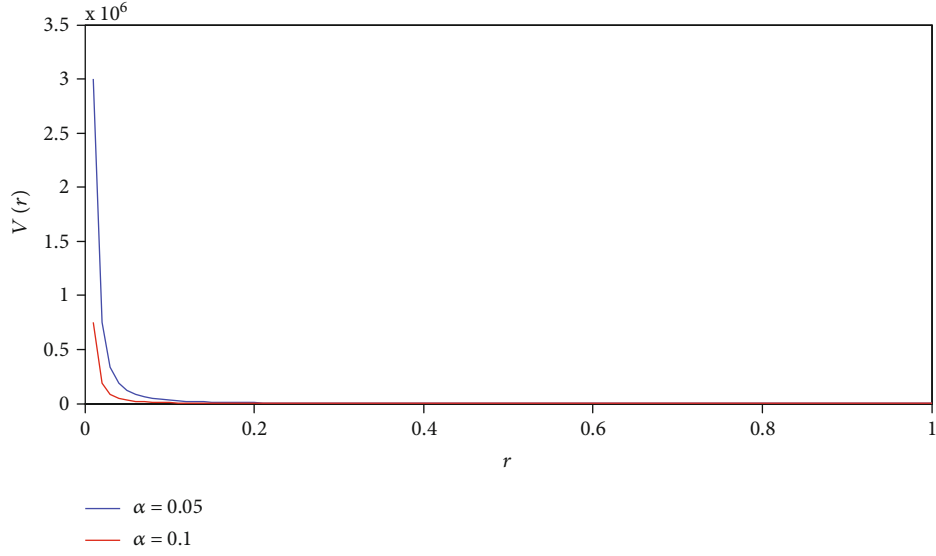
$$B = 2\gamma^2 - \nu^2,$$

FIGURE 4: The Eckart plus Hulthen potential (eV) in terms of $r(A^0)$ for $V_0 = V_1 = 1$ and $\alpha = 0.05, 0.1$.
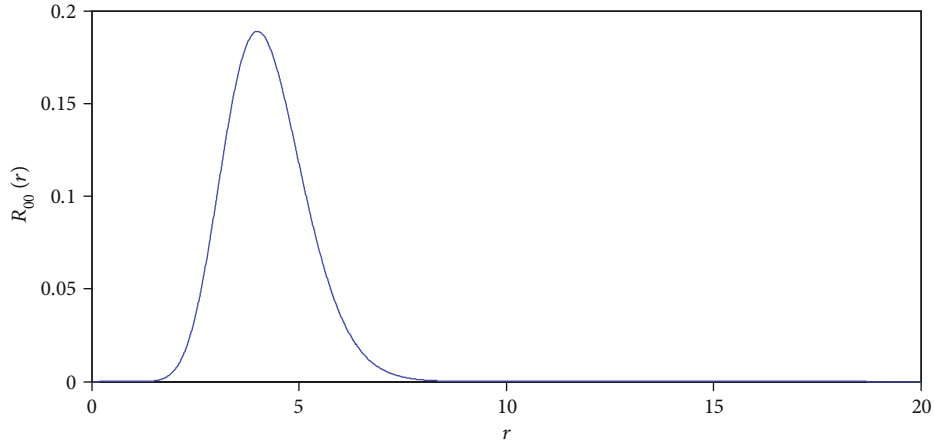

FIGURE 5: Wave function (eV) in terms of $r(A^0)$ of the Eckart plus Hulthen potential for $n = l = 0$, $\alpha = 0.05$, and $V_0 = V_1 = 1$ in atomic units $y = \mu = 1$.

$$v^2 = \frac{(E + m)(4 - V_0)}{4\alpha^2},$$

$$C = \gamma^2 - \beta^2 - \xi^2,$$

$$\xi^2 = \frac{(E + m)(V_1 - V_0)}{4\alpha^2}. \tag{41}$$

Accordingly, the α_i parameters are obtained through Equation (24). Moreover, by using Equation (14) and

$$\delta' = \frac{1}{2}\left(1 + \sqrt{1 + 4v^2 - 4\xi^2}\right), \tag{42}$$

the energy eigenvalue is identified as

$$E^2 - m^2 = -4\alpha^2\left\{\left(\frac{-n^2 - v^2 + 2\beta^2 + 2\xi^2 - (2n+1)\delta'}{2(n + \delta')}\right)^2 + \beta^2 + \xi^2\right\}. \tag{43}$$

The radial wave function is of the following form:

$$R_{nl}(r) = N_{nl} e^{-2\eta\alpha r}\left(1 - e^{-2\alpha r}\right)^{\delta_l} P_n^{(2\eta, 2\delta_l - 1)}\left(1 - 2e^{-2\alpha r}\right)$$
$$= N_{nl}\frac{(2\eta + 1)_n}{n!} e^{-2\eta\alpha r}\left(1 - e^{-2\alpha r}\right)^{\delta_l}{}_2F_1\left(-n, n + 2\eta + 2\delta_l ; 1 + 2\eta ; e^{-2\alpha r}\right). \tag{44}$$

With the variable change $\eta = \sqrt{C}$ and the parameters of Equation (42), we obtain

$$\eta = \frac{1}{2\alpha}\sqrt{-(E+m)(E-m+2(V_1-V_0-1))}. \quad (45)$$

The normalization constant is obtained as

$$N_{nl} = \sqrt{\frac{2\eta\alpha n!(n+\eta+\delta_l)\Gamma(n+2(\eta+\delta_l))}{(n+\delta_l)\Gamma(n+2\eta+1)\Gamma(n+2\delta_l)}} \quad (46)$$

We plot wave function of the Eckart plus Hulthen potential (eV) as a function of $r(A^0)$ for the H_2 diatomic molecule in $n = l = 0$ in Figure 5.

5. Results and Discussion

In this study, we examined the solution of the Klein-Gordon equation for two different potentials. Accordingly, we calculated the energy eigenvalues and normalized wave function for the diatomic molecules for different n and l states through the NU method. In order to solve the Klein-Gordon equation, we utilized the NU method, which can also be used to identify the wave function and energy eigenvalue for any particular potential. However, with certain potentials, the wave equation fails to furnish the boundary conditions of the method.

The parameters related to the spectroscopic constants of these molecules, taken from [19–21] appear in Table 1. Table 2 shows the energy levels for diatomic molecules by using the Morse oscillator potential and the shifted Deng-Fan (sDF) potential. The findings comply well with refs. [23, 24] and also with the energies calculated from AP (amplitude phase) [26, 27].

Based on the results, as the quantum number n increases, the energy value decreases. Furthermore, an increase in l makes the particle less bound. It can further be inferred that in higher dimensions, the energy value decreases. To show the accuracy of our results, we have calculated the eigenvalues numerically for arbitrary n with $l = 0$, $\alpha = 0.05$, and $\alpha = 0.1$. Tables 3 and 4 show the energy levels of the Eckart plus Hulthen potential in atomic units $\hbar = \mu = 1$ with $l = 0$, $\alpha = 0.05$, and $\alpha = 0.1$, respectively. It is observed that as α increases, the energy eigenvalue decreases.

6. Conclusion

Considering the importance of the molecular Deng-Fan potential and the Eckart plus Hulthen potential in molecular physics, chemical physics, molecular spectroscopy, and other related areas, we investigated the bound state solution of the relativistic wave equation. We provided exact solutions of the Klein-Gordon equation for these potentials by means of the Nikiforov-Uvarov (NU) method. We formulated the eigenvalues equation and the corresponding wave function in terms of hypergeometric functions via the NU method within an approximation to the centrifugal potential term.

TABLE 3: The energy levels of the Eckart plus Hulthen potential for several states with $l = 0$, $\alpha = 0.05$, in atomic units $\hbar = \mu = 1$.

V_0	V_1	n	E_{nl}(eV) NU
1	1	0	-1.10125
		1	-1.14085
		2	-1.18559
		3	-1.23510
		4	-1.23906
		5	-1.34726
2	2	0	-1.00125
		1	-1.01056
		2	-1.02800
		3	-1.05246
		4	-1.08371
		5	-1.12063
3	3	0	-1.20005
		1	-1.12267
		2	-1.06792
		3	-1.03138
		4	-1.00976
		5	-1.00061
-1	1	0	-1.78125
		1	-1.84500
		2	-1.91125
		3	-1.98000
		4	-2.05125
		5	-2.12500
-1	2	0	-2.14453
		1	-2.18625
		2	-2.23187
		3	-2.28117
		4	-2.23395
		5	-2.39006

As we know, there is no analytical solution for the radial equation for $l \neq 0$. Therefore, the Klein-Gordon equation is transformed into a differential Schrödinger-like equation through a suitable coordinate transformation. The obtained energies are very close to the energies reported in other studies [19–22]. We preferred to calculate the energy eigenvalue of H_2, CO, LiH, and HCl as diatomic molecules. The main advantage of these molecules is that their spectroscopic values are already known [31]. This feature has made them suitable candidates for working with in other studies, too, e.g., [32]. They also serve different purposes in various aspects of both physics and chemistry [22, 33, 34].

This method of approximation is simple and practical. It can be applied to different quantum models to enhance the accuracy of the energy eigenvalues for some potential models of exponential-type, such as the hyperbolical potential and the Manning-Rosen potential [35, 36]. Our findings in this

TABLE 4: The energy levels of the Eckart plus Hulthen potential for several states with $l = 0$, $\alpha = 0.1$, in atomic units $\hbar = \mu = 1$.

V_0	V_1	n	$E_{nl}(eV)\,NU$
1	1	0	-1.12099
		1	-1.21053
		2	-1.31852
		3	-1.44288
		4	-1.58244
		5	-1.73523
2	2	0	-1.00500
		1	-1.03993
		2	-1.10217
		3	-1.18677
		4	-1.29046
		5	-1.41096
3	3	0	-1.15616
		1	-1.04664
		2	-1.00352
		3	-1.00655
		4	-1.04379
		5	-1.10788
-1	1	0	-1.81378
		1	-1.94636
		2	-2.08894
		3	-2.24151
		4	-2.40409
		5	-2.57667
-1	2	0	-2.16567
		1	-2.25700
		2	-2.36265
		3	-2.48139
		4	-2.61241
		5	-2.75513

section are significant not only in theoretical and chemical physics but also in experimental physics since we obtained general results which are useful for studying nuclear charge radius, spin, and nuclear scattering. In the future, we plan to improve the approximation to solve the Bethe-Salpeter equation with different potentials.

Data Availability

We have not included a data availability statement in our manuscript.

Conflicts of Interest

The authors have not declared any conflict of interest.

References

[1] B. H. Yazarloo, H. Hassanabadi, and S. Zarrinkamar, "Oscillator strengths based on the Möbius square potential under Schrödinger equation," *The European Physical Journal Plus*, vol. 127, no. 5, 2012.

[2] X. Y. Gu and S. H. Dong, "Energy spectrum of the Manning-Rosen potential including centrifugal term solved by exact and proper quantization rules," *Journal of Mathematical Chemistry*, vol. 49, no. 9, pp. 2053–2062, 2011.

[3] S. H. Dong, "A new approach to the relativistic Schrödinger equation with central potential: ansatz method," *International Journal of Theoretical Physics*, vol. 40, no. 2, pp. 559–567, 2001.

[4] H. Hassanabadi, S. Zarrinkamar, and B. H. Yazarloo, "Spectrum of a hyperbolic potential via SUSYQM within the semi-relativistic formalism," *Chinese Journal of Physics*, vol. 50, no. 5, pp. 788–794, 2012.

[5] S. H. Dong and G. H. Sun, "The series solutions of the non-relativistic equation with the Morse potential," *Physics Letters A*, vol. 314, no. 4, pp. 261–266, 2003.

[6] S. H. Dong and X. Y. Gu, "Arbitrary l state solutions of the Schrödinger equation with the Deng-Fan molecular potential," *Journal of Physics: Conference Series*, vol. 96, no. 1, 2008.

[7] G. F. Wei and C. W. Li, "Continuum states of modified Morse potential," *Chinese Physics B*, vol. 19, no. 9, 2010.

[8] G. F. Wei, C. Y. Long, X. Y. Duan, and S. H. Dong, "Arbitraryl-wave scattering state solutions of the Schrödinger equation for the Eckart potential," *Physica Scripta*, vol. 77, no. 3, p. 035001, 2008.

[9] S. H. Dong, "Relativistic treatment of spinless particles subject to a rotating Deng-Fan oscillator," *Communications in Theoretical Physics*, vol. 55, no. 6, pp. 969–971, 2011.

[10] G. F. Wei, X. Y. Liu, and W. L. Chen, "The relativistic scattering states of the Hulthén potential with an improved new approximate scheme to the centrifugal term," *International Journal of Theoretical Physics*, vol. 48, no. 6, pp. 1649–1658, 2009.

[11] G. F. Wei and S. H. Dong, "A novel algebraic approach to spin symmetry for Dirac equation with scalar and vector second Pöschl-Teller potentials," *The European Physical Journal A*, vol. 43, no. 2, pp. 185–190, 2010.

[12] G. F. Wei and S. H. Dong, "Algebraic approach to pseudospin symmetry for the Dirac equation with scalar and vector modified Pöschl-Teller potentials," *Euro physics Letters*, vol. 87, no. 4, p. 40004, 2009.

[13] G. F. Wei and S. H. Dong, "Pseudospin symmetry in the relativistic Manning–Rosen potential including a Pekeris-type approximation to the pseudo-centrifugal term," *Physics Letters B*, vol. 686, no. 4-5, pp. 288–292, 2010.

[14] M. Monemzadeh, N. Tazimi, and P. Sadeghi, "Tetraquarks as diquark–antidiquark bound systems," *Physics Letters B*, vol. 741, pp. 124–127, 2015.

[15] M. Monemzadeh, M. Hadizadeh, and N. Tazimi, "Identification of the mass and stability interval of strong potential in heavy mesons," *International Journal of Theoretical Physics*, vol. 50, no. 3, pp. 737–743, 2011.

[16] M. Radin and N. Tazimi, "Quark-antiquark bound state in momentum-helicity representation," *Physical Review D*, vol. 90, no. 8, 2014.

[17] M. Monemzadeh, N. Tazimi, and S. Babaghodrat, "Calculating masses of pentaquarks composed of baryons and mesons,"

Advances in High Energy Physics, vol. 2016, Article ID 6480926, 4 pages, 2016.

[18] M. C. Zhang, G. H. Sun, and S. H. Dong, "Exactly complete solutions of the Schrödinger equation with a spherically harmonic oscillatory ring-shaped potential," *Physics Letters A*, vol. 374, no. 5, pp. 704–708, 2010.

[19] M. G. Miranda, G. H. Sun, and S. H. Dong, "The solution of the second Pöschl–Teller like potential by Nikiforov-Uvarov method," *International Journal of Modern Physics E*, vol. 19, no. 1, pp. 123–129, 2010.

[20] Z. H. Deng and Y. P. Fan, "A potential function of diatomic molecules," *Journal of Shandong University (Natural Science)*, vol. 1, 1957.

[21] G. F. Wei, Z. Z. Zhen, and S. H. Dong, "The relativistic bound and scattering states of the Manning-Rosen potential with an improved new approximate scheme to the centrifugal term," *Central European Journal of Physics*, vol. 7, no. 1, pp. 175–183, 2009.

[22] W. C. Qiang and S. H. Dong, "Analytical approximations to the solutions of the Manning–Rosen potential with centrifugal term," *Physics Letters A*, vol. 368, no. 1-2, pp. 13–17, 2007.

[23] S. M. Ikhdair, "Rotation and vibration of diatomic molecule in the spatially-dependent mass Schrödinger equation with generalized q-deformed Morse potential," *Chemical Physics*, vol. 361, no. 1-2, pp. 9–17, 2009.

[24] S. M. Ikhdair, "Effective Schrödinger equation with general ordering ambiguity position-dependent mass Morse potential," *Molecular Physics*, vol. 110, no. 13, pp. 1415–1428, 2012.

[25] E. Castro, J. L. Paz, and P. Martin, "Analytical approximations to the eigenvalues of the Morse potential with centrifugal terms," *Journal of Molecular Structure: THEOCHEM*, vol. 769, no. 1-3, pp. 15–18, 2006.

[26] H. J. Korsch and H. Laurent, "Milne's differential equation and numerical solutions of the Schrodinger equation. I. Bound-state energies for single- and double-minimum potentials," *Journal of Physics B: Atomic and Molecular Physics*, vol. 14, no. 22, pp. 4213–4230, 1981.

[27] T. Yano, Y. Ezawa, T. Wada, and H. Ezawa, "Can Milne's method work well for the Coulomb-like potentials ?," *Journal of Computational and Applied Mathematics*, vol. 152, no. 1-2, pp. 597–611, 2003.

[28] M. Abramowitz and I. A. Stegun, *Handbook of mathematical functions*, Dover publication, New York, NY, 1972.

[29] S. M. Ikhdair, "An approximate κ state solutions of the Dirac equation for the generalized Morse potential under spin and pseudospin symmetry," *Journal of Mathematical Physics*, vol. 52, no. 5, p. 052303, 2011.

[30] A. D. Alhaidari, "Solution of the Dirac equation with position-dependent mass in the Coulomb field," *Physics Letters A*, vol. 322, no. 1-2, pp. 72–77, 2004.

[31] K. J. Oyewumi, B. J. Falaye, C. A. Onate, O. J. Oluwadare, and W. A. Yahya, "Thermodynamic properties and the approximate solutions of the Schrödinger equation with the shifted Deng-Fan potential model," *Molecular Physics*, vol. 112, no. 1, pp. 127–141, 2014.

[32] J. A. Kunc and F. J. Gordillo-Vazquez, "Rotational-vibrational levels of diatomic molecules represented by the Tietz-Hua rotating oscillator," *The Journal of Physical Chemistry A*, vol. 101, no. 8, pp. 1595–1602, 1997.

[33] B. J. Falaye, K. J. Oyewumi, T. T. Ibrahim, M. A. Punyasena, and C. A. Onate, "Bound state solutions of the Manning-Rosen potential," *Canadian Journal of Physics*, vol. 91, no. 1, pp. 98–104, 2013.

[34] K. J. Oyewumi and K. D. Sen, "Exact solutions of the Schrödinger equation for the pseudoharmonic potential: an application to some diatomic molecules," *Journal of Mathematical Chemistry*, vol. 50, no. 5, pp. 1039–1059, 2012.

[35] S. M. Ikhdair and R. Sever, "Improved analytical approximation to arbitrary l-state solutions of the Schrödinger equation for the hyperbolical potential," *Annalen der Physik*, vol. 18, no. 4, pp. 189–197, 2009.

[36] M. R. Setare and S. Haidari, "Bound states of the Dirac equation with some physical potentials by the Nikiforov-Uvarov method," *Physica Scripta*, vol. 81, no. 1, 2009.