Bound States of the Relativistic Rotating Deng-Fan Oscillator Potential

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Abstract

The generalized Morse or Deng-Fan Potential describes diatomic molecular energy spectra and electromagnetic transitions. We solve the Klein-Gordon (K-G) equation for Deng-Fan Potential in arbitrary $N$-dimension and use an improved approximation scheme to the centrifugal term. By using the generalized parametric Nikiforov-Uvarov (NU) method, we obtain the energy eigenvalues and corresponding wave functions in closed forms. The effect of potential parameters and the dimension $N$ on the energy eigenvalues is numerically discussed.

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Keywords: Klein-Gordon equation; rotating Deng-Fan oscillator potential; generalized Nikiforov-Uvarov method

1. Introduction

In the twenty last years, great attentions paid to solve K-G and Dirac equations for various quantum systems. Also, the exact analytic solutions of the wave functions are only possible for certain potentials such as Coulomb, harmonic, Mie-type and pseudoharmonic potentials [1-5]. The analytic exact solutions of the wave functions with some exponential-type are possible for $l = 0$ cases and approximation solutions have to be used to the centrifugal terms such as Pekeris approximation [6] and the approximation scheme suggested by Greene and Aldrich [7]. Many authors used
different methods to study the exactly and approximately solvable Schrödinger, K-G and Dirac equations in one-, 3- and/or any \( N \)-dimensional cases for different potentials [8-25].

The Deng-Fan potential suggested by Deng and Fan is rotating potential defined by [26]

\[
V(r) = D \left(1 - \frac{b}{e^{a r} - 1}\right)^2, \quad b = e^{a r} - 1,
\]

(1)

where \( r \in (0, \infty) \) and \( D, r_e \) and \( a \) denote the dissociation energy, equilibrium internuclear distance and range of the potential well, respectively. The Deng-Fan Potential describes diatomic molecular energy spectra and electromagnetic transitions [27].

Dong and Gu approximately presented the bound state solutions of the Schrödinger equation with the rotating Deng-Fan molecular potential [28]. Mesa et al. studied the bound state spectrum of Deng-Fan potential by an \( so(2,2) \) symmetry algebra and calculated the Frank-Gondon factors for electromagnetic transition between rovibrational levels based on different electronic states [27]. Very recently, Ikhdair solved the Dirac equation for the generalized Morse potential with arbitrary spin-orbit quantum number \( \kappa \) [29].

In this paper, we investigate K-G equation for Deng-Fan potential in arbitrary \( N \)-dimension, by using an improved approximation scheme to deal with the centrifugal term. We use the generalized parametric NU method to obtain energy eigenvalues and corresponding eigenfunctions. Thus, this paper is arranged as follows: in section 2, we give a brief introduction to K-G equation in \( N \)-dimension. In section 3, The NU method is briefly introduced. The generalized parametric NU method is displayed in appendix A. In section 4, we solve hyperradial K-G equation with Deng-Fan potential by the mentioned method. Some numerical results are given in this section, too. Finally, our conclusions are given in section 5.

2. K-G equation in \( N \)-dimension

In spherical coordinates, the K-G equation with vector potential \( V(r) \), and scalar one \( S(r) \), is written as \([\hbar = c = 1]\)

\[
-\Delta_N \psi_{nlm}(r, \Omega_N) = \left[ (E_{nl} - V(r))^2 - (m - S(r))^2 \right] \psi_{nlm}(r, \Omega_N),
\]

(2)

with

\[
\Delta_N = \nabla_N^2 = \frac{1}{r^{N-1}} \frac{\partial}{\partial r} \left( r^{N-1} \frac{\partial}{\partial r} \right) - \frac{\Lambda_N^2(\Omega_N)}{r^2},
\]

(3)

where \( E_{nl} \), \( \Lambda_N^2(\Omega_N) \) and \( \Omega_N \) are the energy eigenvalues, a generation of the centrifugal barrier for \( N \)-dimension and the angular coordinates, respectively. The eigenvalues of the \( \Lambda_N^2(\Omega_N) \) are given by

\[
\Lambda_N^2(\Omega_N) \psi_i^{(m)}(\Omega_N) = l(l + D - 2) \psi_i^{(m)}(\Omega_N),
\]

(4)
where $Y_i^m(\Omega_N)$ is the hyperspherical harmonics. Using separation variables method with the wave function $\psi_{nml}(r, \Omega_N) = \frac{R_{n,l}(r)}{r} Y_i^m(\Omega_N)$, Eq. (2) reduces to

$$\frac{d^2}{dr^2} + E_{nl} - V^2(r) - 2E_{nl}V(r) - \frac{(N + 2l - 1)(N + 2l - 3)}{4r^2} R_{n,l}(r) = 0.$$  \hspace{1cm} (5)

When vector potential $V(r)$ is equal to the scalar potential $S(r)$, lead us to obtain a Schrödinger-like equation as

$$\frac{d^2}{dr^2} + \varepsilon^2 - 2(E_m - m)V(r) - \frac{(N + 2l - 1)(N + 2l - 3)}{4r^2} R_{n,l}(r) = 0, \hspace{1cm} (6)$$

where $\varepsilon^2 = E_m^2 - m^2$. Because of the centrifugal term in above equation, we can not solve it exactly. By using the following improved new approximation scheme to the centrifugal term near the minimum point $r = r_c$, as [29]

$$\frac{1}{r^2} \approx a^2 \left[ d_0 + \frac{1}{e^2 - 1} + \frac{1}{(e^2 - 1)^2} \right], \hspace{1cm} (7)$$

where $d_0 = \frac{1}{12}$, Eq. (6) can be solvable and with substitution of Eq. (1), it becomes as follows

$$\frac{d^2}{dr^2} + \varepsilon^2 - 2(E_m - m)D \left(1 - \frac{b}{e^2 - 1} \right)^2 - \frac{a^2(N + 2l - 1)(N + 2l - 3)}{4} \left[ d_0 + \frac{1}{e^2 - 1} + \frac{1}{(e^2 - 1)^2} \right] R_{n,l}(r) = 0. \hspace{1cm} (8)$$

To solve Eq. (8), we use the and its generalized parametric NU method.

### 3. Generalized Parametric Nikiforov-Uvarov method

To solve second order differential equations, the Nikiforov-Uvarov method can be used with an appropriate coordinate transformation $s = s(r)$ [30]

$$\psi''_n(s) + \frac{\tilde{\tau}(s)}{\sigma(s)} \psi'_n(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} \psi_n(s) = 0, \hspace{1cm} (9)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. The following equation is a general form of the Schrödinger-like equation written for any potential [31]
According to the Nikiforov-Uvarov method, the eigenfunctions and eigenenergy function become, respectively

\[
\psi(s) = s^{\alpha_2} \left(1 - \alpha_3 s\right)^{-\alpha_3 \alpha_4} \alpha_4 P_n^{(\alpha_0, 1)} \left(1 - 2\alpha_3 s\right),
\]

\[
\alpha_3 n - (2n + 1)\alpha_4 + (2n + 1)\left(\sqrt{\alpha_0} + \alpha_3 \sqrt{\alpha_6}\right) + n(n + 1)\alpha_6 + \alpha_7 + 2\alpha_3 \alpha_4 + 2\sqrt{\alpha_5} \alpha_4 = 0,
\]

where

\[
\alpha_4 = \frac{1}{2}(1 - \alpha_1), \quad \alpha_5 = \frac{1}{2}(\alpha_2 - 2\alpha_3),
\]

\[
\alpha_6 = \alpha_2^2 + \xi_1, \quad \alpha_7 = 2\alpha_4 \alpha_4 - \xi_2,
\]

\[
\alpha_8 = \alpha_2^2 + \xi_3, \quad \alpha_9 = \alpha_3 \alpha_7 + \alpha_3^2 \alpha_8 + \alpha_6,
\]

and

\[
\alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8}, \quad \alpha_{11} = \alpha_2 - 2\alpha_5 + 2\left(\sqrt{\alpha_0} + \alpha_3 \sqrt{\alpha_8}\right),
\]

\[
\alpha_{12} = \alpha_4 + \sqrt{\alpha_8}, \quad \alpha_{13} = \alpha_5 - \left(\sqrt{\alpha_0} + \alpha_3 \sqrt{\alpha_8}\right).
\]

In some problems \(\alpha_3 = 0\). For this type of problems when

\[
\lim_{\alpha_3 \to 0} P_n^{\left(\alpha_0, 1\right)} \left(1 - \alpha_3 s\right) = L_n^{\alpha_0^{-1}} \left(\alpha_4 s\right),
\]

and

\[
\lim_{\alpha_3 \to 0} \left(1 - \alpha_3 s\right)^{-\alpha_3} = e^{\alpha_3 s},
\]

the solution given in Eq. (9) becomes as [31]

\[
\psi(s) = s^{\alpha_2} e^{\alpha_3 s} L_n^{\alpha_0^{-1}} \left(\alpha_4 s\right).
\]

4. Solution of hyperradial K-G equation with Deng-Fan potential

To solve Eq. (8), by using an appropriate transformation as \(s = \frac{1}{e^w - 1}\), we rewrite it as follows

\[
\frac{d^2 R_{nl}(r)}{dr^2} + \frac{1 + 2s}{s(1+s)} \frac{dR_{nl}(r)}{dr} + \frac{1}{s^2(1+s)^2} \left[-\xi_0 s^2 + \xi_2 s - \xi_3\right] R_{nl}(r) = 0,
\]

where
Comparing Eq. (14) and Eq. (A1), we can easily obtain the coefficients $\alpha_i$ ($i = 1, 2, 3$) as follows
$$
\alpha_1 = 1, \quad \alpha_2 = 2, \quad \alpha_3 = -1.
$$
(20)
The values of coefficients $\alpha_i$ ($i = 4, 5, \ldots, 13$) are found from Eqs. (13-14) and displayed in table 1. By using Eq. (12), we can obtain the closed form energy eigenvalues of the Deng-Fan potential as
$$
2(n + 1)(\sqrt{\xi_1} + \sqrt{\xi_2} + \sqrt{\xi_3} + 4 - \sqrt{\xi_4}) + 2\sqrt{\xi_1}(\sqrt{\xi_2} + \sqrt{\xi_3} + 4) - \xi_5 - 2\xi_3 - (n^2 + 3n + 2) = 0.
$$
(21)
Some numerical results are given in table 2 and figures 1-3. The potential parameters are taken from Ref. [28] and $m = 1 \text{fm}^{-1}$. In table 2, we calculated bound state energy with $r_c = 0.4 \text{fm}$ for various $a$ and $N$. In fig 1, we plotted energy eigenvalues as a function of range of the potential well $a$, $N = 3$ and $r_c = 0.4 \text{fm}$. We see that when $a$ increase, the energy increase too and when $n$ and/or $l$ increase the $a$ affect more (green line). In fig 2, the effect of equilibrium inter-nuclear distance $r_e$, $N = 3$ and $a = 0.05 \text{fm}^{-1}$ is shown. When $r_e$ increase the energy decrease and it has more effect on states with higher $n$ and/or $l$ (for example; compare yellow and green lines in fig. 2). Finally, in fig. 3, we show the effect of dimension on the energy levels. When $N$ increase the energy increase too, but it has more effect on lower states (compare yellow and green lines in fig. 2) and it can be seen that the energy eigenvalues decrease from $N = 1$ to 3 and next increase.

To find corresponding wave functions, referring to table 1 and Eq. (11), we get the radial wave functions as
$$
R_{nl}(s) = N_{nl}s^{\xi_1}(1 + s)^{2\sqrt{\xi_1} + \xi_2 + 4}P_n^{(2\sqrt{\xi_1} - 2\sqrt{\xi_1 + \xi_2 + 4})}(1 + 2s),
$$
(22)
where $N_{nl}$ is normalization constant.

4. Conclusions

In this work, by using an improved approximation scheme to the centrifugal barrier term, we obtained approximate solutions of the generalized Morse or Deng-Fan potential by using the generalized parametric NU method. The bound state
eigenvalues and corresponding wave functions are given in their closed forms and some numerical are given in table 2 and figures 1-3.

References

Table 1. The specific values for the parametric constants necessary for the energy eigenvalues and eigenfunctions

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<th>constant</th>
<th>Analytic value</th>
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<td>$\alpha_{10}$</td>
<td>$1 + 2\sqrt{\xi_3}$</td>
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<td>$\alpha_{11}$</td>
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<td>$\alpha_{12}$</td>
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<td>$\alpha_{13}$</td>
<td>$2 - 2(\sqrt{\xi_1 + \xi_2 + \xi_3 + 4} - \sqrt{\xi_3})$</td>
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Table 2: The bound state energy eigenvalues in unit of $\mu m^{-1}$ of the Deng-Fan potential for several values of $N$, $a$, $n$, and $l$ with $r_c = 0.4$.

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<th>(N)</th>
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<th>(E_{0,0})</th>
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Fig. 1: Energy behavior versus $a$ for $N = 3$ and various $n, l$ s.

Fig. 2: Energy behavior versus $r_e$ for $N = 3$ and various $n, l$ s.
Fig. 3: Energy behavior versus $N$ for various $n_l$ s.