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Analytical Solution of the D-Dimensional Klein-Gordon Equation for Dan-Fan Molecular Potential Using AIM

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Abstract

In this article, the D-dimensional Klein-Gordon equation within the framework of improved Greene-Aldrich approximations scheme for Deng-Fan molecular potential is solved for s-wave and arbitrary angular momenta. The energy eigenvalues and corresponding wave functions are obtained in an exact analytical manner with the help of asymptotic iteration method.

Keywords: Deng-Fan molecular potential, improved Greene-Aldrich approximation scheme, asymptotic iteration method (AIM)
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1 Introduction

The Klein-Gordon equation plays an important role in explaining the interacting behavior of spinless particles with different physical potentials [1, 2]. Recently, many researchers have investigated the problem of finding solutions to various special potentials of the D-dimensional Klein-Gordon equation [3, 4, 5, 6, 7, 8, 9, 10]. In the literature, Nikiforov-Uvarov method [11, 12, 13], asymptotic iteration method [14], Point-Cannonical transformation [15], Lie algebraic method [16], Laplace transform approach [17, 18], Factorization method[19], etc.

The Deng-Fan potential [20, 21], is widely used in molecular physics and quantum chemistry. The Deng-Fan molecular potential is:

$$V(r) = D_e\left[1 - \frac{A}{e^{\alpha r} - 1}\right]^2, \qquad A = e^{\alpha r_e} - 1 \tag{1}$$

where r_e is the molecular bond length, D_e is the dissociation energy, r is the inter-nuclear distance and α the range of the potential well.

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While studying behavior of Deng-Fan molecular potential within the Klein-Gordon equation, we use modified approach of Greene-Aldrich [22] and use some simple constraints within AIM.

Our work is assembled as: the AIM is briefed in section 2 to make it accessible. Section 3 considers the D-dimensional Klein-Gordon equations that describe the Dan-Fan molecular potential along with the modified Green-Aldrich approximation. The solutions are extracted in section 4. Section 5 contains the concluding remarks.

2 The Asymptotic Iteration Method:

Let us chose the second-order differential equation of the form :

$$g_n''(u) = \varrho_0(u)g_n'(u) + \sigma_0(u)g_n(u) \tag{2}$$

with sufficiently differentiable variables, $\sigma_0(u)$ and $\varrho_0(u)(\neq 0)$.
Differentiation of equation (2) for u, gives

$$g_n'''(u) = \varrho_1(u)g_n'(u) + \sigma_1(u)g_n(u) \tag{3}$$

in which

$$\begin{aligned} \varrho_1(u) &= \varrho_0'(u) + \sigma_0(u) + \varrho_0^2(u), \\ \sigma_1(u) &= \sigma_0'(u) + \sigma_0(u)\varrho_0(u). \end{aligned} \tag{4}$$

The second derivative of (2) results

$$g_n^4(u) = \varrho_2(u)g_n'(u) + \sigma_2(u)g_n(u), \tag{5}$$

Where

$$\begin{aligned} \varrho_2(u) &= \varrho_1'(u) + \sigma_1(u) + \varrho_0(u)\varrho_1(u), \\ \sigma_2(u) &= \sigma_1'(u) + \sigma_0(u)\varrho_1(u). \end{aligned} \tag{6}$$

Equation (2) can be extended up to $(k+1)^{th}$ and $(k+2)^{th}$ derivatives, where $k = 1, 2, 3, \ldots$ and obtain

$$\begin{aligned} g_n^{(k+1)}(u) &= \varrho_{k-1}(u)g_n'(u) + \sigma_{k-1}(u)g_n(u), \\ g_n^{(k+2)}(u) &= \varrho_k(u)g_n'(u) + \sigma_k(u)g_n(u), \end{aligned} \tag{7}$$

Where

$$\begin{aligned} \varrho_k(u) &= \varrho_{k-1}'(u) + \sigma_{k-1}(u) + \varrho_0(u)\varrho_{k-1}(u), \\ \sigma_k(u) &= \sigma_{k-1}'(u) + \sigma_0(u)\varrho_{k-1}(u). \end{aligned} \tag{8}$$

By equation (7), we have

$$\frac{d}{du}\ln[g_n^{(k+1)}(u)] = \frac{g_n^{(k+2)}(u)}{g_n^{(k+1)}(u)} = \frac{\varrho_k(u)[g_n'(u) + \frac{\sigma_k(u)}{\varrho_k(u)}g_n(u)]}{\varrho_{k-1}(u)[g_n'(u) + \frac{\sigma_{k-1}(u)}{\varrho_{k-1}(u)}g_n(u)]}. \tag{9}$$

For sufficiently large k. For asymptotic nature, let

$$\frac{\sigma_k(u)}{\varrho_k(u)} = \frac{\sigma_{k-1}(u)}{\varrho_{k-1}(u)} = \alpha(u) \tag{10}$$

And (9) deduces

$$\frac{d}{du}\ln[g_n^{(k+1)}(u)] = \frac{\varrho_k(u)}{\varrho_{k-1}(u)}, \tag{11}$$

This gives

$$g_n^{(k+1)}(u) = C_1 exp\left(\int \frac{\varrho_k(u)}{\varrho_{k-1}(u)}du\right) = C_1\varrho_{k-1}(u)exp\left(\int [\alpha(u)+\varrho_0(u)]du\right), \tag{12}$$

where C_1 is the integration constant and the right hand side of (12) is obtained by using (10) and (11). By inserting (12) into (7), the first-order differential equation is obtained as

$$g_n'(u) + \alpha(u)g_n(u) = C_1 exp\left(\int [\alpha(u)+\varrho_0(u)]du\right). \tag{13}$$

So,

$$g_n(u) = exp\left(-\int^u \alpha(u_1)du_1\right)[C_2 + C_1\int^u exp\left(\int^{u_1}[\varrho_0(u_2)+2\alpha(u_2)]du_2\right)du_1] \tag{14}$$

The condition to terminate the method is

$$\Delta_k(u) = \varrho_k(u)\sigma_{k-1}(u) - \varrho_{k-1}(u)\sigma_k(u) = 0, \tag{15}$$

where k shows the iteration number (the radial quantum number $n = k$, for our study). The energy eigenvalues are obtained from the roots of (15).

The general solution of (2) is given by (14). The first part of (14) gives us the polynomial solutions that are convergent and physical, whereas the second part of (14) gives us non-physical solutions that are divergent. For the square integrable solutions, the coefficient of the second part (C_1) should be zero. Thus, found wave function generator:

$$g_n(u) = C_2 exp\left(-\int^u \frac{\sigma_n(u_1)}{\varrho_n(u_1)}du_1\right), \tag{16}$$

where n represents the principal quantum number.

3 The D-dimensional Klein-Gordon equation

The time independent D-dimensional Klein-Gordon equation (in atomic units $\hbar = c = \mu = 1$,) is[23],

$$\nabla_D^2\Psi(r,\Omega_D) + \left[\left(E - V(r)\right)^2 - \left(M + S(r)\right)^2\right]\Psi(r,\Omega_D) = 0 \tag{17}$$

Here, **M**, **E**, $\mathbf{V}(\mathbf{r})$ and $\mathbf{S}(\mathbf{r})$ represent particle mass, energy, vector potential and scalar potential. The operator ∇_D^2 as [24],

$$\nabla_D^2 = \frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right) - \frac{L_D^2(\Omega_D)}{r^2} \tag{18}$$

with ground angular momentum $L_D^2(\Omega_D)$ [25] given by $L_D^2(\Omega_D) = -\Sigma_{i\geq j}^{D}(L_{ij}^2)$ with $L_{ij}^2 = x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i}$ for x_i $(i = 1,2,\ldots,D)$.

We define

$$\Psi(r,\Omega_D) = r^{\frac{(D+1)}{2}} R_{nl}(r) Y_{lm}(\Omega_D) \tag{19}$$

where $Y_{lm}(\Omega_D)$is the generalized spherical harmonic function. $L_2^D Y_{lm}(\Omega_D) = l(l+D-2)Y_{lm}(\Omega_D)$ is the eigenvalues equation. Therefore, the radial part can be reduced as:

$$\frac{d^2R_{nl}(r)}{dr^2} + \Bigg[\Big(E^2 - M^2\Big) - 2\Big(MS(r) + EV(r)\Big) \\ + V^2(r) - S^2(r) - \frac{(2l+D-3)(2l+D-1)}{4r^2}\Bigg] R_{nl}(r) = 0 \tag{20}$$

Assuming $V(r) = S(r)$, equation (12) becomes

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[\Big(E^2 - M^2\Big) - 2V(r)(M+E) - \frac{(2l+D-3)(2l+D-1)}{4r^2}\right] R_{nl}(r) = 0 \tag{21}$$

The term $\frac{1}{r^2}$ reveals a singularity which we remove with the help of an improved Greene-Aldrich approximation scheme by

$$\frac{1}{r^2} \approx \alpha^2 \left[D_0 + \frac{e^{-\alpha r}}{\Big(1 - e^{-\alpha r}\Big)^2}\right] \tag{22}$$

As per literature, this scheme is better than the Greene and Aldrich [22] approximation scheme.

Using equation(1) and equation(22) in equation(21), we have

$$\frac{d^2R_{nl}(r)}{dr^2} + \Bigg[\Big(E^2 - M^2\Big) - 2(M+E)D_e\Big[1 - \frac{A}{e^{\alpha r} - 1}\Big]^2 - \\ \frac{(2l+D-3)(2l+D-1)}{4}\left[D_0 + \frac{\alpha^2 e^{-\alpha r}}{\Big(1 - e^{-\alpha r}\Big)^2}\right] R_{nl}(r) = 0 \tag{23}$$

By simplification, the equation reduces to

$$\frac{d^2R_{nl}(r)}{dr^2} - \left[\frac{(\epsilon^2 + \gamma^2 D_0)(1 - e^{-\alpha r})^2 - \beta^2 e^{-\alpha r}(1 - e^{-\alpha r}) + \eta^2 e^{-2\alpha r} + \gamma^2 e^{-\alpha r}}{\Big(1 - e^{-\alpha r}\Big)^2}\right] R_{nl}(r) = 0 \tag{24}$$

where, $-\epsilon^2 = \frac{E^2 - M^2 - 2D_e(M+E)}{\alpha^2}$, $\beta^2 = \frac{4D_e A(M+E)}{\alpha^2}$, $\eta^2 = \frac{2D_e A^2(M+E)}{\alpha^2}$, and $\gamma^2 = \frac{(2l+D-3)(2l+D-1)}{4}$.

4 Solutions:

To have a solvable form of equation (9), we launch a new variable $s = e^{-\alpha r}$ and obtain

$$\frac{d^2R(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dR}{ds} - \frac{1}{s^2(1-s)^2}\Bigg[(\epsilon^2 + \gamma^2 D_0 + \beta^2 + \eta^2)s^2 - \\ (2\epsilon^2 + 2\gamma^2 D_0 + \beta^2 - \gamma^2)s + (\epsilon^2 + \gamma^2 D_0)\Bigg] R(s) = 0 \tag{25}$$

For reasonable physical wave function, $R(s)=0$ at $s=0$ when $r\to\infty$ and $R(s)=0$ at $s=1$ when $r\to 0$. So, the wave function takes the form:

$$R(s)=s^{\mu}(1-s)^{\nu}g_n(s) \tag{26}$$

Where, $\mu=\sqrt{\epsilon^2+\gamma^2 D_0}$ and $\nu=\frac{1}{2}+\sqrt{\frac{1}{4}+\eta^2+\gamma^2}$.
And $R'(s)$ and $R''(s)$ becomes

$$R'(s)=\left[f_n'(s)+\Big(\frac{\mu}{s}-\frac{\nu}{(1-s)}\Big)g_n(s)\right]s^{\mu}(1-s)^{\nu}$$

$$R''(s)=\left[g_n''(s)+2[\frac{\mu}{s}-\frac{\nu}{(1-s)}]g_n'(s)+\left(\Big(\frac{\mu}{s}-\frac{\nu}{(1-s)}\Big)^2-\frac{\mu}{s^2}-\frac{\nu}{(1-s)^2}\right)g_n(s)\right]s^{\mu}(1-s)^{\nu}$$

Now inserting these values of $R(s)$, $R'(s)$ and $R''(s)$ into equation(25), we found:

$$g_n''(s)=\Big[\frac{(2\mu+2\nu+1)s-(2\mu+1)}{s(1-s)}\Big]g_n'(s)+\Big[\frac{(\mu+\nu)^2-(\mu^2+\beta^2+\gamma^2)}{s(1-s)}\Big]g_n(s) \tag{27}$$

Comparing equation(27) and equation(2), the values of $\varrho_0(s)$ and $\sigma_0(s)$ can be obtained and the values of $\varrho_k(s)$ and $\sigma_k(s)$ can be calculated using the recursion relation (8). This gives,

$$\varrho_0(s)=\frac{(2\mu+2\nu+1)s-(2\mu+1)}{s(1-s)}$$

$$\sigma_0(s)=\frac{(\mu+\nu)^2-(\mu^2+\beta^2+\gamma^2)}{s(1-s)}$$

$$\varrho_1(s)=\frac{1}{s^2(1-s)^2}\Bigg[[3(\mu+\nu+1)^2-1+(\mu^2+\beta^2+\gamma^2)]s^2+[(\mu+\nu)^2-$$
$$4(\mu+\nu+1)(2\mu+1)-(\mu^2+\beta^2+\gamma^2)]s+2(\mu+1)(2\mu+1)\Bigg]$$

$$\sigma_1(s)=\frac{1}{s^2(1-s)^2}\Bigg[(\mu+\nu)^2-(\mu^2+\beta^2+\gamma^2)][(2\mu+2\nu+3)s-2(\mu+1)\Bigg] \tag{28}$$

Using these in equation (15), the first value of $\Delta_1(s)$ is obtained as

$$\Delta_1(s)=\frac{[(\mu+\nu)^2-(\mu^2+\beta^2+\gamma^2)][(\mu+\nu+1)^2-(\mu^2+\beta^2+\gamma^2)]}{s^2(1-s)^2} \tag{29}$$

According to termination condition, the value of $\Delta_1(s)$ should be zero which gives the first value of μ_0 as $\mu_0=\frac{-\nu^2+\beta^2+\gamma^2}{2\nu}$. Similarly,

$$\Delta_2(s)=\varrho_2(s)\sigma_1(s)-\varrho_1(s)\sigma_2(s)=0\Longrightarrow\mu_1=\frac{-(\nu+1)^2+\beta^2+\gamma^2}{2(\nu+1)}$$

$$\Delta_3(s) = \varrho_3(s)\sigma_2(s) - \varrho_2(s)\sigma_3(s) = 0 \Longrightarrow \mu_2 \frac{-(\nu+2)^2+\beta^2+\gamma^2}{2(\nu+2)}, \tag{30}$$

...Clearly,

$$\mu_n = \frac{-(\nu+n)^2+\beta^2+\gamma^2}{2(\nu+n)};\ n = 0,1,2,3,.................... \tag{31}$$

Inserting the values of μ and ν in equation(31), we obtain

$$-\epsilon_n^2 = \gamma^2 D_0 - \frac{1}{4}\left[\frac{-\chi^2+\beta^2+\gamma^2}{\chi}\right]^2 \tag{32}$$

where, $\chi = n + \frac{1}{2} + \sqrt{\frac{1}{4} + \eta^2 + \gamma^2}$

Fixing the values of $\epsilon, \beta, \eta, \gamma$ the approximate energy eigenvalue is:

$$E_{nl} \approx 2D_e + \frac{\alpha^2(2l+D-1)(2l+D-3)D_0}{2M} - \frac{\alpha^2}{8M}\left[\frac{-\zeta^2 + \frac{8MAD_e}{\alpha^2} + \frac{(2l+D-1)(2l+D-3)}{4}}{\zeta}\right]^2 \tag{33}$$

Where, $\zeta = n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{4MAD_e}{\alpha^2} + \frac{(2l+D-1)(2l+D-3)}{4}}$

To obtain the corresponding eigenfunction, we rearrange the equation(27) as:

$$s(1-s)\frac{d^2 g_n(s)}{ds^2} + [(2\mu+1)-(2\mu+2\nu+1)s]\frac{dg_n(s)}{ds} - \left[(\mu+\nu)^2 - (\mu^2+\beta^2+\gamma^2)\right]g_n(s) = 0 \tag{34}$$

This is the Gauss hypergeometric equation and the solutions are the Gauss hypergeometric functions [26]:

$$g_n(s) =_2 F_1(p,q;c;s) \tag{35}$$

in which,

$$\begin{aligned} p &= (\mu+\nu) - \sqrt{\mu^2+\beta^2+\eta^2} \\ q &= (\mu+\nu) + \sqrt{\mu^2+\beta^2+\eta^2} \\ c &= 2\mu+1 \end{aligned} \tag{36}$$

One the other hand, $p = -n$ by equation(31).

Therefore,

$$R(s) = s^{\sqrt{\epsilon^2+\gamma^2 D_0}}(1-s)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\eta^2+\gamma^2}}_{\ 2}F_1(-n, n+2(\mu+\nu); 2\mu+1; s) \tag{37}$$

This is the wave function.

5 Conclusion

This article uses the improved Green-Aldrich approximation for the eccentric terms to presents the solution of the D-dimensional Klein-Gordon equation having the same scalar and vector potentials as the molecular Dan-Fan potential. The work continued here with the help of AIM by converting the target equation into a form $g_n''(s) = \varrho_0(s)g_n'(s) + \sigma_0(s)g_n(s)$ through iteration of $\sigma_0(s)$ and $\varrho_0(s)$. The energy eigenvalues has been obtained in exact analytical form and the eigen functions (wave functions) has been obtained in gamma functions and Gauss hypergeometric functions.

6 Declarations

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Competing Interests

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Ethical Approval

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Authors's Contributions

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