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Review Paper

Analytical Solutions of the D-dimensional Klein-Gordon equation for Deng-Fan molecular potential via Factorization method

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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 potential is solved for s-wave and arbitrary angular momenta. The energy eigenvalues and corresponding wave functions are obtained in an exact analytical manner.
Keywords: *Deng-Fan potential, improved Greene-Aldrich approximation scheme, Factorization method.*
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I. Introduction :

The Klein-Gordon equation plays an important role in describing the behavior of relativistic spinless particles [1, 2] with various physical potentials. Recently, the problem of finding analytical solutions of D-dimensional Klein-Gordon equation for a number of special potentials has been studied by numerous Scientists [3, 4, 5, 6, 7, 8, 9, 10]. The solutions are also crucial in quantum soluble systems. Several methods have been adopted in literature such as 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.

In this article, the approximate solutions of Klein-Gordon equation in D-dimensions is obtained for Deng-Fan potential. The Deng-Fan [20, 21], is an intermolecular potential and widely applied to molecular physics and quantum chemistry. The Deng-Fan molecular potential is:

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

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

To investigate the behaviour of Deng-Fan molecular potential within the frame work of Klein-Gordon equation I use an improved Greene-Aldrich approximation [22] and applying some simple constraints such that the equation can be solved by Factorization method.

My work is organized as follows: - In section II, the D-dimensional Klein-Gordon equation is presented considering the Deng-Fan molecular potential as well as improved Greene-Aldrich approximation. In section III, the energy eigenvalues and corresponding wave functions are obtained for the D-dimensional Klein-Gordon equation by using Factorization method. Section IV contains the concluding remark.

II. The Klein-Gordon equation in D-dimensions:

The time independent D-dimensional Klein-Gordon equation in the atomic units $\hbar$ = c = μ = 1, may be written as [23],

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

where M denotes the particle mass, E is the energy, V(r) and S(r) are vector and scalar potentials respectively. The D-dimensional Laplacian operator $\boldsymbol{\nabla_D^2}$ is given by [24],

$$\boldsymbol{\nabla_D^2 = r^{1-D}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right) + \frac{L_D^2(\Omega_D)}{r^2}} \qquad (3)$$

Where, $L_2^D(\Omega_D)$ is the ground angular momentum [25]. In addition, we know that $\frac{L_D^2(\Omega_D)}{r^2}$ is a generalization of the centrifugal barrier for the D-dimensional space and involves angular coordinates Ω_D and the eigenvalues of $L_2^D(\Omega_D)$ [24]. $L_2^D(\Omega_D)$ is a partial differential operator on the unit space S^{D-1} define analogously to a three-dimensional angular momentum [25] as $L_D^2(\Omega_D) = -\sum_{i\geq j}^{D}(L_{ij}^2)$, where $L_{ij}^2 = x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i}$ for all Cartesian component xi of the D-dimensional vector $(x_1, x_2, \ldots\ldots, x_D)$.
To eliminate the first order derivative, the total wave function may be defined as

$$\Psi(r,\Omega_D) = r^{\frac{(D+1)}{2}} R_{nl}(r) Y_{lm}(\Omega_D) \qquad (4)$$

Where, $Y_{lm}(\Omega_D)$ is the generalized spherical harmonic function. The eigenvalues equation for the generalized angular momentum operator is given by $L_2^D(\Omega_D) = l(l + D - 2)Y_{lm}(\Omega_D)$. With this, we can write the radial part of the D-dimensional Klein-Gordon equation as follows:

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[(E^2 - M^2) - 2\big(MS(r) + EV(r)\big) + V^2(r) - S^2(r) - \frac{(2l + D - 1)(2l + D - 3)}{4r^2}\right] R_{nl}(r) = 0 \qquad (5)$$

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

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[(E^2 - M^2) - 2V(r)(M + E) - \frac{(2l + D - 1)(2l + D - 3)}{4r^2}\right] R_{nl}(r) = 0 \qquad (6)$$

The solution for the above equation with $l \neq 0$ is mainly depending on replacing the orbital centrifugal term of singularity with the help of a suitable approximation scheme. The approximation scheme used in this article to deal with the centrifugal term is an improved Greene-Aldrich approximation scheme given by:

$$\frac{1}{r^2} \approx \alpha^2\left[D_0 + \frac{e^{-\alpha r}}{(1 - e^{-\alpha r})^2}\right] \qquad (7)$$

It has been shown extensively in literature that this approximation scheme approximates the centrifugal barrier better than the well-known Greene and Aldrich [22] approximation scheme. In the limiting case when $\alpha r \rightarrow 1$, the value of the dimensionless constant $D_0 = \frac{1}{12}$
and the screening parameter α approaches zero, Eqn. (7) reduces to $\frac{1}{r^2}$.

Inserting the potential function and the modified centrifugal term as given in Eqn. (1) and Eqn. (7) respectively in Eqn. (6), we have

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[(E^2 - M^2) - 2D_e(M + E)\left(1 - \frac{A}{e^{\alpha r} - 1}\right)^2 - \frac{(2l + D - 1)(2l + D - 3)}{4}\left[D_0 + \frac{e^{-\alpha r}}{(1 - e^{-\alpha r})^2}\right]\right] R_{nl}(r) = 0 \qquad (8)$$

By simplification, the equation reduces to

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[\frac{(\epsilon^2 + \gamma^2 D_0)(1 - e^{-\alpha r})^2 - \beta^2 e^{-\alpha r}(1 - e^{-\alpha r}) + \eta^2 e^{-2\alpha r} + \gamma^2 e^{-\alpha r}}{(1 - e^{-\alpha r})^2}\right] R_{nl}(r) = 0 \qquad (9)$$

where, I have used the notations,

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

III. Solutions of the D-dimensional Klein-Gordon equation:

In order to solve Eqn. (9) by the Factorization method, we need to recast it into a solvable form. To do so, I introduce a new variable s = e−αr and Eqn. (9) takes the form

$$\frac{d^2R(s)}{ds^2} + \frac{(1 - s)}{s(1 - s)}\frac{dR(s)}{ds} - \frac{1}{s^2(1 - s)^2}[(\epsilon^2 + \gamma^2 D_0 + \beta^2 + \eta^2)s^2 - (2\epsilon^2 + 2\gamma^2 D_0 + \beta^2 - \gamma^2)s + (\epsilon^2 + \gamma^2 D_0)]R(s) = 0 \qquad (10)$$

The wave function should satisfy the boundary conditions, i.e. R(s) = 0 at s = 0 when r →∞ and R(s) = 0 at s = 1 when r → 0 . Therefore, the reasonable physical wave function is of the form:

$$R(s) = s^{\mu}(1-s)^{\nu}f(s) \tag{11}$$

Where, $\mu = \sqrt{\boldsymbol{\epsilon^2}+\boldsymbol{\gamma^2 D_0}}$ and $\nu = \frac{1}{2}+\sqrt{\frac{1}{4}+\eta^2+\boldsymbol{\gamma^2}}$.

substituting Eqn. (11) into Eqn. (10) one can easily obtain the following hypergeometric equation:

$$s(1-s)\frac{d^2f(s)}{ds^2}+[(2\mu+1)-(2\mu+2\nu+1)s]\frac{df(s)}{ds}-[(\mu+\nu)^2-(\mu^2+\boldsymbol{\beta^2}+\boldsymbol{\gamma^2})]f(s) \tag{12}$$

The solutions of the Eqn. (12) are the Gauss hypergeometric functions:

$$f(s) = {}_2F_1(a,b;c;s) \tag{13}$$

Where,

$$a = (\mu+\nu) - \sqrt{\mu^2+\boldsymbol{\beta^2}+\boldsymbol{\gamma^2}}$$
$$b = (\mu+\nu) + \sqrt{\mu^2+\boldsymbol{\beta^2}+\boldsymbol{\gamma^2}}$$
$$c = 2\mu+1 \tag{14}$$

The solutions should satisfy the finiteness condition and this suggests the quantum condition:

$$(\mu+\nu) - \sqrt{\mu^2+\boldsymbol{\beta^2}+\boldsymbol{\gamma^2}} = -n, \qquad where, n = 0,1,2,\ldots \tag{15}$$

From this one can get,

$$\epsilon^2 = -\gamma^2 D_0 + \frac{1}{4}\left[\frac{-\eta^2-\boldsymbol{\beta^2}+\boldsymbol{\chi^2}}{\chi}\right]^2 \tag{16}$$

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

This constitutes the energy eigenvalue equation for Deng-Fan molecular potential and the approximate energy eigenvalue (by putting the values of notations $\epsilon, \beta, \eta, \gamma$) is of the form:

$$E_{nl} \approx 2D_e\alpha^2 + \frac{\alpha^2(\boldsymbol{2l+D-1})(\boldsymbol{2l+D-3})D_0}{8} - \frac{\alpha^2}{2M}\left[\frac{\xi^2-\frac{4MA^2D_e}{\alpha^2}-\frac{8MAD_e}{\alpha^2}}{\xi}\right]^2 \tag{17}$$

Where, $\xi = n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{8MA^2D_e}{\alpha^2}+\frac{(\boldsymbol{2l+D-1})(\boldsymbol{2l+D-3})}{4}}$.

The corresponding wave function is obtained as

$$R(s) = s^{\sqrt{\boldsymbol{\epsilon^2}+\boldsymbol{\gamma^2 D_0}}}(1-s)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\eta^2+\boldsymbol{\gamma^2}}}\ {}_2F_1(-n, n+2(\mu+\nu); 2\mu+1; s) \quad (18$$

IV. Conclusions :

In this article, the solutions of the D-dimensional Klein-Gordon equation with equal scalar and vector potentials for the Deng-Fan molecular potential using an improved Greene-Aldrich approximation to the centrifugal term via Factorization method. The relativistic energy eigenvalues are obtained and the corresponding wave functions in terms of the hypergeometric functions are presented.

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