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Research Article

The Nonrelativistic Scattering States of the Deng-Fan Potential

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The approximately analytical scattering state solution of the Schrodinger equation is obtained for the Deng-Fan potential by using an approximation scheme to the centrifugal term. Energy eigenvalues, normalized wave functions, and scattering phase shifts are calculated. We consider and verify two special cases: the $l = 0$ and the s-wave Hulthén potential.

1. Introduction

One of the interesting problems in quantum mechanics is to investigate the energy spectra and the wavefunctions of a quantum system under different potentials because one can obtain all the necessary information regarding the quantum system under consideration. In order to understand the studied quantum system completely, we should study the bound states and the scattering states for a given quantum system. Among various potential models, we consider the Deng-Fan potential. In 1957, Deng and Fan [1] introduced Deng-Fan potential in an attempt to find a more suitable diatomic potential to describe the vibrational spectrum. The Deng-Fan potential is a molecular potential, and it is qualitatively similar to the Morse potential. In the description of the motion of nucleons this potential is applicable. As the forthcoming (2) reveals, this potential, in some ranges of the potential perimeter, is very similar to the Kratzer potential. The Deng-Fan potential is consistent with quantum requirements and can be a suitable choice to study physical systems besides the Coulomb or linear terms. This potential has been investigated by some authors under different wave equations of quantum mechanics [2–5]. In [3], arbitrary l state solutions of the Schrödinger equation with the Deng-Fan molecular potential is reported. Dong in [2] obtained the energy spectra of the Klein-Gordon equation under the equal scalar and vector potentials by using a proper approximation to the centrifugal term. To deal with the wave equations in quantum mechanics such as Klein-Gordon [6], Dirac [7], Duffin-Kemmer-Petiau [8], and Schrodinger [3] equations different methods have been used; these methods include the supersymmetry (SUSY) method [9], Nikiforov-Uvarov method [10], the quantization rules [11], series expansion [12], and ansatz method [13].

Here, we report solutions of the scattering states of Schrodinger equation for the Deng-Fan potential for any l states. The reasons for which we write this paper are as follows. Firstly, we have not yet found the scattering states related to this potential. Secondly, theoretical prediction of many properties of diatomic molecules requires the knowledge of the radial wavefunctions of scattering states and the phase shifts. In [14] the authors have obtained the properties of scattering state solutions of the Klein-Gordon equation for a Coulomb like scalar plus vector potentials. The analytical scattering state solutions of the l-wave Schrodinger equation for the Eckart potential is given in [15]. The scattering states of Schrodinger and the Klein-Gordon equations under different potentials are reported in [16–19].

The rest of this paper is organized as follow. In Section 2, we obtain the solutions of scattering states. The normalized radial wave functions of scattering states and the calculation formula of phase shifts are presented. In Section 3, we consider and verify two special cases: the $l = 0$ and the s-wave Hulthén potential. And finally, our conclusion is given in Section 4.

2. Scattering States of the Arbitrary l-Wave Schrodinger Equation

The radial Schrodinger equation has the form

$$\left[\frac{d^2}{dr^2} - \frac{2\mu}{\hbar^2}V(r) - \frac{l(l+1)}{r^2} + \frac{2\mu E_{n,l}}{\hbar^2}\right] R_{n,l}(r) = 0, \quad (1)$$

where μ and $\hbar$ are the reduced mass and the Planck's constant, respectively. Here, we consider the Deng-Fan potential

$$V(r) = V_0 + \frac{V_1}{e^{\alpha r} - 1} + \frac{V_2}{(e^{\alpha r} - 1)^2}, \quad (2)$$

where r denotes the hyper radius and V_0, V_1, V_2, and α are constant coefficients. Substitution of (2) into (1) gives

$$\begin{gathered}\left[\frac{d^2}{dr^2} - \frac{2\mu}{\hbar^2}\left(V_0 + \frac{V_1}{e^{\alpha r} - 1} + \frac{V_2}{(e^{\alpha r} - 1)^2}\right)\right. \\ \left. -\frac{l(l+1)}{r^2} + \frac{2\mu E_{n,l}}{\hbar^2}\right] R_{n,l}(r) = 0.\end{gathered} \quad (3)$$

To get rid of the centrifugal term, we make use of the elegant approximation [2]

$$\begin{gathered}\frac{1}{r^2} \approx \alpha^2\left(d_0 + \frac{e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{e^{-2\alpha r}}{(1 - e^{-\alpha r})^2}\right), \\ d_0 = \frac{1}{12}, \quad \alpha = 0.15.\end{gathered} \quad (4)$$

Equation (3) changes into

$$\left\{\frac{d^2}{dr^2} - A\frac{e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} - B\frac{e^{-\alpha r}}{1 - e^{-\alpha r}} + C\right\} R_{n,l}(r) = 0, \quad (5)$$

where

$$\begin{aligned} A &= \frac{2\mu V_2}{\hbar^2} + l(l+1)\alpha^2, \\ B &= \frac{2\mu V_1}{\hbar^2} + l(l+1)\alpha^2, \\ C &= \frac{2\mu E_{n,l}}{\hbar^2} - \frac{2\mu V_0}{\hbar^2} - l(l+1)d_0\alpha^2. \end{aligned} \quad (6)$$

Introducing $s = 1 - \exp(-\alpha r)$ brings (5) as

$$\begin{gathered}\left\{s(1-s)\frac{d^2}{ds^2} - s\frac{d}{ds} - \frac{A}{\alpha^2}\frac{1-s}{s} + \frac{C}{\alpha^2}\frac{s}{1-s} - \frac{B}{\alpha^2}\right\} \\ \times R_{n,l}(s) = 0.\end{gathered} \quad (7)$$

To proceed on, we choose

$$R_{n,l}(s) = s^{\mu'}(1-s)^{v'} g_{n,l}(s). \quad (8)$$

Substitution of (8) into (7) leads to

$$\begin{gathered}\left\{s(1-s)\frac{d^2}{ds^2} + \left(2\mu' - \left(1 + 2v' + 2\mu'\right)s\right)\frac{d}{ds}\right. \\ \left. -\left(\mu'^2 + v'^2 + 2\mu' v' - \frac{A - B - C}{\alpha^2}\right)\right\} g_{n,l}(s) = 0.\end{gathered} \quad (9)$$

Equation (9) can be written as

$$\left\{s(1-s)\frac{d^2}{ds^2} + \left(c' - \left(1 + a' + b'\right)s\right)\frac{d}{ds} - a'b'\right\} g_{n,l}(s) = 0. \quad (10)$$

Equation (10) is the hypergeometric equation, and its solution is the hypergeometric function, so we have

$$g_{n,l}(s) = {}_2F_1\left(a', b', c'; s\right), \quad (11)$$

where

$$\begin{aligned} a' &= \frac{1}{2}\left(2\mu' + 2v' + \sqrt{\frac{A - B - C}{\alpha^2}}\right) \\ &= \frac{1}{2}\left(2\mu' - 2i\sqrt{\frac{C}{\alpha^2}} + \sqrt{\frac{4}{\alpha^2}(A - B - C)}\right), \\ b' &= \frac{1}{2}\left(2\mu' + 2v' - \sqrt{\frac{A - B - C}{\alpha^2}}\right) \\ &= \frac{1}{2}\left(2\mu' - 2i\sqrt{\frac{C}{\alpha^2}} - \sqrt{\frac{4}{\alpha^2}(A - B - C)}\right), \\ c' &= 2\mu', \\ v'^2 &= -\frac{C}{\alpha^2} \Longrightarrow v' = -ik, \quad k = \sqrt{\frac{C}{\alpha^2}}, \\ \mu'^2 - \mu' &= -\frac{A}{\alpha^2} \Longrightarrow \mu' = \frac{1}{2}\left(1 + \sqrt{1 + \frac{4A}{\alpha^2}}\right). \end{aligned} \quad (12)$$

Therefore the total wavefunction of the system is

$$\begin{aligned} R_{n,l}(s) &= s^{\mu'}(1-s)^{v'} g_{n,l}(s) \\ &= s^{\mu'}(1-s)^{v'} {}_2F_1\left(a', b', c'; s\right). \end{aligned} \quad (13)$$

Or equivalently ($s = 1 - e^{-\alpha r}$)

$$R_{n,l}(r) = N_{n,l}(1 - e^{-\alpha r})^{\mu'} e^{i\alpha k r} {}_2F_1\left(a', b', c';\ 1 - e^{-\alpha r}\right). \quad (14)$$

To obtain a finite solution, a' or b' must be a negative integer. This gives the following equality:

$$\frac{1}{2}\left(2\mu' - 2i\sqrt{\frac{2\mu E_{n,l}}{\hbar^2\alpha^2} - \frac{2\mu V_0}{\hbar^2\alpha^2} - l(l+1)d_0} + \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(V_2 - V_1 + V_0) - \frac{2\mu E_{n,l}}{\hbar^2\alpha^2} + l(l+1)d_0}\right) = -n \quad (n = 0, 1, 2, \ldots), \tag{15}$$

where the energy eigenvalue equation can be found from the previous equation.

Here, to obtain the normalized constant and phase shifts we recall the following properties of hypergeometric function:

$${}_2F_1(a, b; c;\; 0) = 1, \tag{16a}$$

$${}_2F_1(a, b; c; s) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \times {}_2F_1(a, b; a+b-c+1; 1-s) + (1-s)^{c-a-b}\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} \times {}_2F_1(c-a, c-b; c-a-b+1; 1-s). \tag{16b}$$

By using (16a) and (16b) ${}_2F_1(a', b', c';\; 1 - e^{-\alpha r})$ for $r \to \infty$ can be written as

$${}_2F_1\left(a', b', c';\; 1 - e^{-\alpha r}\right) = \Gamma(c')\left[\frac{\Gamma(c' - a' - b')}{\Gamma(c' - a')\Gamma(c' - b')} + \frac{\Gamma(a' + b' - c')}{\Gamma(a')\Gamma(b')}e^{-\alpha(c' - a' - b')r}\right]. \tag{17}$$

By inserting the following relations in the previous equation

$$c' - a' - b' = 2ik = \left(a' + b' - c'\right)^*, \quad c' - a' = b'^*, \quad c' - b' = a'^*. \tag{18}$$

We obtain

$${}_2F_1\left(a', b', c';\; 1 - e^{-\alpha r}\right) = \Gamma(c')\left[\frac{\Gamma(c' - a' - b')}{\Gamma(c' - a')\Gamma(c' - b')} + \left[\frac{\Gamma(c' - a' - b')}{\Gamma(c' - a')\Gamma(c' - b')}\right]^* e^{-2i\alpha kr}\right]. \tag{19}$$

By taking $\Gamma(c' - a' - b')/\Gamma(c' - a')\Gamma(c' - b') = |\Gamma(c' - a' - b')/\Gamma(c' - a')\Gamma(c' - b')|e^{i\delta'}$ and inserting in (19) we arrive at

$${}_2F_1\left(a', b', c';\; 1 - e^{-\alpha r}\right) = \Gamma(c')\left|\frac{\Gamma(c' - a' - b')}{\Gamma(c' - a')\Gamma(c' - b')}\right| e^{-i\alpha kr} \times \left[e^{i(\alpha kr + \delta')} + e^{-i(\alpha kr + \delta')}\right]. \tag{20}$$

Therefore, we have the asymptotic form of the formula (14) for $r \to \infty$

$$R_{n,l}(r) = 2N_{n,l}\Gamma(c')\left|\frac{\Gamma(c' - a' - b')}{\Gamma(c' - a')\Gamma(c' - b')}\right| \times \sin\left(\alpha kr + \frac{\pi}{2} + \delta'\right). \tag{21}$$

By comparing (21) with the boundary condition [20] $r \to \infty \Rightarrow u(\infty) \to 2\sin(kr - l\pi/2 + \delta_l)$ phase shifts and the normalized constant can be given by

$$\delta_l = \frac{\pi}{2} + \frac{l\pi}{2} + \delta' = \frac{\pi}{2} + \frac{l\pi}{2} + \arg\left[\Gamma\left(c' - a' - b'\right)\right] - \arg\left[\Gamma\left(c' - a'\right)\right] - \arg\left[\Gamma\left(c' - b'\right)\right], \quad N_{n,l} = \frac{1}{\Gamma(c')}\left|\frac{\Gamma(c' - a')\Gamma(c' - b')}{\Gamma(c' - a' - b')}\right|. \tag{22}$$

3. Discussion

In this section we study two special cases. First, we discuss the special case $l = 0$. In this case, we have

$$A = \frac{2\mu V_2}{\hbar^2}, \qquad B = \frac{2\mu V_1}{\hbar^2}, \qquad C = \frac{2\mu E_{n,l}}{\hbar^2} - \frac{2\mu V_0}{\hbar^2},$$
$$\upsilon' = -i\sqrt{\frac{2\mu E_{n,l}}{\hbar^2\alpha^2} - \frac{2\mu V_0}{\hbar^2\alpha^2}}, \qquad \mu' = \frac{1}{2}\left(1 + \sqrt{1 + \frac{8\mu V_2}{\alpha^2\hbar^2}}\right). \tag{23}$$

Therefore, the results which is obtained in the previous section are reduced to the those of the exact solutions of s-wave scattering state for the Deng-Fan potential as follows:

$$\delta_l = \frac{\pi}{2} + \arg\left[\Gamma\left(2i\sqrt{\frac{2\mu}{\hbar^2\alpha^2}(E_n - V_0)}\right)\right]$$
$$- \arg\left[\Gamma\left(\mu' + i\sqrt{\frac{2\mu}{\hbar^2\alpha^2}(E_n - V_0)} - \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(V_0 - V_1 + V_2 - E_n)}\right)\right]$$
$$- \arg\left[\Gamma\left(\mu' + i\sqrt{\frac{2\mu}{\hbar^2\alpha^2}(E_n - V_0)} + \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(V_0 - V_1 + V_2 - E_n)}\right)\right],$$

$$N = \frac{1}{\Gamma\left(1 + \sqrt{1 + \frac{8\mu V_2}{\alpha^2\hbar^2}}\right)} * \left|\Gamma\left(\mu' + i\sqrt{\frac{2\mu}{\hbar^2\alpha^2}(E_n - V_0)} - \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(V_0 - V_1 + V_2 - E_n)}\right) \times \Gamma\left(\mu' + i\sqrt{\frac{2\mu}{\hbar^2\alpha^2}(E_n - V_0)} + \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(V_0 - V_1 + V_2 - E_n)}\right) \times \left(\Gamma\left(2i\sqrt{\frac{2\mu}{\hbar^2\alpha^2}(E_n - V_0)}\right)\right)^{-1}\right|. \quad (24)$$

Second, we consider the case of $V_0 = V_2 = 0$ in which the Deng-Fang potential reduces to the Hulthen potential. In the case of $l = 0$, we have

$$A = 0, \qquad B = \frac{2\mu V_1}{\hbar^2}, \qquad C = \frac{2\mu E_{n,l}}{\hbar^2},$$
$$\mu' = 2, \qquad \upsilon' = -i\sqrt{\frac{2\mu E_{n,l}}{\hbar^2\alpha^2}}. \quad (25)$$

The results given in (22) are reduced to

$$\delta_l = \frac{\pi}{2} + \arg\left[\Gamma\left(2i\sqrt{\frac{2\mu E_n}{\hbar^2\alpha^2}}\right)\right] - \arg\left[\Gamma\left(1 + i\sqrt{\frac{2\mu E_n}{\hbar^2\alpha^2}} - \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(-V_1 - E_n)}\right)\right] - \arg\left[\Gamma\left(1 + i\sqrt{\frac{2\mu E_n}{\hbar^2\alpha^2}} + \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(-V_1 - E_n)}\right)\right],$$

$$N = \left|\Gamma\left(1 + i\sqrt{\frac{2\mu E_n}{\hbar^2\alpha^2}} - \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(-V_1 - E_n)}\right) \times \Gamma\left(1 + i\sqrt{\frac{2\mu E_n}{\hbar^2\alpha^2}} + \sqrt{\frac{2\mu}{\hbar^2\alpha^2}(-V_1 - E_n)}\right) \times \left(\Gamma\left(2i\sqrt{\frac{2\mu E_n}{\hbar^2\alpha^2}}\right)\right)^{-1}\right| \quad (26)$$

which are same as the s-wave scattering state for the Hulthén potential [20] if we choose $\alpha = 1/\beta$, $V_1 = -A/\kappa\beta^2$.

4. Conclusion

Due to the application of the Deng-Fan potential for theoretical physicists especially for molecular system, we have discussed the approximate bound and scattering state solutions of the Schrodinger equation for the Deng-Fan potential. We have obtained the energy eigenvalues, normalized wave functions, and scattering phase shifts by using an approximation for the centrifugal term. We should mention that from the relation of the scattering phase shifts and the general theory of the partial-wave method one can obtain the scattering amplitude. Also, we have studied two special cases for $l = 0$ and the s-wave of the Hulthén potential which is a special case of the Deng-Fan potential. Results are useful in quantum mechanics and particle physics.

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