

Analytical Solution Of Schrödinger Equation With Mie-Type Potential Using Factorisation Method

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ABSTRACT

we have obtained the analytical solution of Schrödinger wave equation with Mie – type potential using factorization method. We have also obtained energy eigenvalues of our potential and the corresponding wave function using an ansatz and then compare the result to standard Laguerre's differential equation. Under special cases our potential model reduces two well known potentials such as Coulomb and the Kratzer Feus potentials.

KEYWORDS

Factorization method, Mie-type potential, Schrödinger equation. PACS numbers: 03.65.Ge, 03.65.Pm, 03.65-w

1. INTRODUCTION

It is well known in quantum mechanics that a total wave function provides implicitly all relevant information about the behaviour of a physical system, hence, if it is exactly solvable for a given potential, the wave function can describe such system completely [1-5]. The exact solution to Schrodinger equation plays a major role in quantum mechanical systems, meanwhile, this solution is only possible for several selected potentials and approximation methods are frequently used to arrive at the solution [6]. Generally, there are few main methods use to study the solutions of quantum mechanical systems. One of them is the analytical method which is basically the variational method and perturbation theory, but because of some inadequacies of this method in addressing some quantum mechanical problems since the problem of suitable choice of initial and convergence with respect to perturbation theory, numerical methods have been introduced [3].

Correspondingly, various methods have been developed to find the approximate solution to Schrödinger equation. Such methods include standard method, path integral approach, invariance method [4], Nikiforov-Uvarov method [1] and others [5]. In this work, we use the factorization method to obtain the exact solution to Schrödinger equation using Mie – type potential. However, with appropriate choice of parameters, our potential model can be reduced to Kratzer –Feus potential and coulomb potential . Meanwhile, the Kratzer potential is amongst the most attractive physical potentials as it contains a degeneracy removing inverse square term besides the common

coulomb term [7-13]. Analytical and Exact solution of the Schrodinger equation are very important because of the understanding of physics that can be brought out from such solutions [14-18].

2. FACTORIZATION METHOD

The factorization method [19] is a way of solving differential equations by change of variables. In spherical coordinate, the Schrödinger wave equation is given as:

$$\frac{-\hbar^2}{2\mu} \nabla^2 \psi(r) + V(r) \psi(r) = E\psi(r) \quad (1)$$

Where μ is the reduce mass and the Laplacian operation ∇^2 in spherical coordinate is given by

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} + (r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial}{\partial \theta}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \quad (2)$$

Let the wave function be

In order to solve Eq. (1), we assume total wave function to be a product of three functions and write it as

$$\Psi(r) = \Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad (3)$$

where $R(r)$ is the radial part, $\Theta(\theta)$ is the angular part and $\Phi(\phi)$ is the azimuthal part of the wave function. Substituting Eqs. (2) and (3) into Eq. (1) we obtain the following equations

Substituting equation (4) into (3)

$$\frac{d^2 \Phi(\phi)}{d\phi^2} + m_l^2 \Phi = 0 \quad (4)$$

$$\frac{1}{\sin(\theta)} \frac{d}{d\theta} (\sin \theta \frac{d\Theta(\theta)}{d\theta}) + [\lambda - \frac{m_l^2}{\sin^2 \theta}] \Theta(\theta) \quad (5)$$

$$\frac{1}{r^2} \frac{d}{dr} (r^2 \frac{dR}{dr}) + \frac{2\mu r^2}{\hbar^2} [E - V_{eff}] R(r) \quad (6)$$

Where

$\lambda = l(l + 1)$, and l is the angular momentum quantum number

$V_{eff} = V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}$ is the effective potential and $\frac{l(l+1)\hbar^2}{2\mu r^2}$ is the centrifugal term. m_l is the magnetic quantum number.

The solutions of Eqs. (4) and (6) are well known. Eq. (5) results in Legendre polynomials. Their product $Y_l^{m_l}(\theta, \phi)$ called spherical harmonics or Condon-Shortley phase is which is documented in literatures [20]

$$Y_l^{m_l}(\theta, \phi) = \Theta(\theta) \Phi(\phi) \quad (7)$$

The solution of Eq. (5) depends mainly on $V(r)$, the potential of the system. Some potential can be solved exactly but in most cases only approximate solution can be obtained for cases for non-vanishing centrifugal term. The energies of the system are also obtained from Eq. (6)

3. SOLUTION OF THE RADIAL PART

The potential of our study is a Mie-Type potential given by [21]

$$V(r) = -\frac{A}{r} + \frac{B}{r^2} + C \quad (8)$$

This potential is useful in describing diatomic molecules. The Mie type potential possesses the general features of the true interaction energy [22, 23]. The Mie-Type and Pseudo-harmonic potentials are the two special kinds of exactly solvable Power-law and inverse power law potentials other than the Coulombic and harmonic oscillator[22]. The potential can reduce to two special cases. The potential reduces to Coulomb-like potential if we set B=C=0

$$V(r) = -\frac{A}{r} \quad (9)$$

and to Kratzer-Feus if we set C=0.

$$V(r) = -\frac{A}{r} + \frac{B}{r^2} \quad (10)$$

Putting this potential of Eq.(8) into the Schrodinger wave equation of Eq.(6), we get

$$\frac{d^2R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \frac{2\mu}{\hbar^2} \left[\left(E + \frac{A}{r} - \frac{B}{r^2} - C \right) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R_n(r) = 0 \quad (11)$$

Recently, Ikot et al. [14] used the ansatz

$$R_n(r) = W_0(r) \left[1 + \frac{\ln}{W_0(r)} (1 + W_0(r)) \right] L(r) \quad (12)$$

By the use of Taylor's series expansion Eq. (12) can be reduced to

$$R(r) \cong 2W_0(r)L(r) \quad (13)$$

Substituting Eq. (12) into Eq. (11) we obtain

$$rL''(r) + \left[\frac{2r}{W_0 + \ln(1+W_0)} \left(W_0' + \frac{W_0'}{1+W_0} \right) + 2 \right] L'(r) + \left[\frac{1}{W_0 + \ln(1+W_0)} \left(W_0'' + \frac{W_0''}{1+W_0} - \frac{W_0'^2}{(1+W_0)^2} \right) + 2W_0 + \ln 1 + W_0' + W_0' + W_0' + W_0 + 2\mu r \hbar^2 E - C + Ar - Br^2 - ll + 12\mu r^2 Lr = 0 \quad (14)$$

Where the primes are derivatives with respect to r and the argument of $W_0(r)$ has been suppressed.

The standard Laguerre's differential equation is defined as [20]

$$rL''(r) + (1 + \alpha - \beta r)L'(r) + \left[(2n - m)\beta - m(\alpha + m) \frac{1}{r} \right] L(r) = 0 \quad (15)$$

The $L(r)$ are the Laguerre's polynomial.

Comparing Eqs. (14) and (15) we obtain

$$\frac{2r}{W_0 + \ln(1+W_0)} \left(W_0' + \frac{W_0'}{1+W_0} \right) + 2 = 1 + \alpha - \beta r \quad (16)$$

Performing a simple integration on Eq. (16) we obtain

$$\ln \frac{W_0^2}{1+W_0} = \ln r^{\alpha-1} - \beta r + D \quad (17)$$

Where D is a constant of integration.

This equation can be simplified further to obtain

$$W_0(r) = r^{\alpha-1} e^{-\beta r} \quad (18)$$

The wave function of the Mie-Type potential can be obtained by

Substituting Eq. (18) into Eq. (13) as

$$R(r) = 2r^{\alpha-1} e^{-\beta r} L_n(r), \quad (19)$$

Where $L_n(r)$ is the Laquerre's polynomial as given by the Rodrigues formula as [20]

$$L(r) = \frac{a_{n,m}(\alpha, \beta)}{r^{\alpha+\frac{m}{2}} e^{-\beta r}} \left(\frac{d}{dr} \right)^{n-m} \left(r^{n+\alpha} e^{-\beta r} \right) \quad (20)$$

The exact wave function is obtained by substituting Eq. (18) into Eq. (12) as

$$R(r) = N_n r^{\alpha-1} e^{-\beta r} [1 + r^{1-\alpha} e^{\beta r} \ln(1 + r^{\alpha-1} e^{-\beta r})] L_n(r) \quad (21)$$

Where N_n is the normalization constant.

The total wave function can be written from Eq. (3) as

$$\Psi_{nlm} = N_n r^{\alpha-1} e^{-\beta r} [1 + r^{1-\alpha} e^{\beta r} \ln(1 + r^{\alpha-1} e^{-\beta r})] L_n(r) Y_l^{m_l}(\theta, \phi) \quad (22)$$

3.1 Eigen values:

In order to obtain the eigenvalues, we shall use the approximate value of the eigenfunction. We insert Eq. (19) into Eq. (13) to get

$$rL''(r) + 2(\alpha - 1 - \beta r + 1)L'(r) + \left\{ \left[\left(\frac{2\mu E}{\hbar^2} - \frac{2\mu C}{\hbar^2} + \beta^2 \right) r - \left(2\beta(\alpha - 1) + 2\beta - \frac{2\mu A}{\hbar^2} \right) \right] + \alpha - 1 \right\} L(r) - 2\mu B \hbar^2 - l(l+1)1rLr = 0 \quad (23)$$

Comparing Eqs. (23) and (15) we obtain the following set of equations

$$\frac{2\mu E}{\hbar^2} - \frac{2\mu C}{\hbar^2} + \beta^2 = 0 \quad (24)$$

$$\frac{2\mu A}{\hbar^2} - 2\beta(\alpha - 1) - 2\beta = (2n - m)\beta \quad (25)$$

$$(\alpha - 1)(\alpha - 2) + 2(\alpha - 1) - \frac{2\mu B}{\hbar^2} - l(l + 1) = -m(\alpha + m) \quad (26)$$

Combining equations (24) and (25) gives

$$E_n = C - \frac{2\mu A^2}{\hbar^2 [2n - m + 2\alpha]^2} \quad (28)$$

Equation (28) gives the energy spectrum. From Eq. (26) we obtain

$$\alpha = \frac{-(m-1) \pm \sqrt{(1+m)(1-3m) + 4\left[l(l+1) + \frac{2\mu B}{\hbar^2}\right]}}{2} \quad (29)$$

3.2 Special Cases:

Kratzer-Fues Potential: if we set $C = 0$ in equation (8) we obtain Kratzer-Fues potential and using this parameter in Eq.(28), we obtain the energy eigenvalues of this system as

$$E_{nlm}^{KF} = -\frac{2\mu A^2}{\hbar^2 [2n - m + 2\alpha]^2} \quad (30)$$

Coulomb Potential: If we set $B = C = 0$ in equation (8), we obtain Coulomb potential and using $B=0$ in Eq. (29) and $C=0$ in Eq.(28), we obtain the energy spectrum of coulomb potential as

$$E_{nlm}^c = \frac{-2\mu A^2}{\hbar^2 [2n - m + 2\alpha_1]^2}, \quad (31)$$

$$\text{where, } \alpha_1 = \frac{-(m-1) \pm \sqrt{(1+m)(1-3m) + 4l(l+1)}}{2}. \quad (32)$$

3. CONCLUSION

In this paper, we have studied the analytic solution of the Schrödinger equation for Mie-type potential using factorization method. We have obtained the wave function using an ansatz and also obtain the corresponding energy spectrum. We have showed that under special cases our results reduce to two well known potentials: Coulomb and Kratzer-Fues potentials by making proper adjustments to constant A, B and C. However, the Mie-type potential as discuss by Agboola [21] is a diatomic potential that can be studied using polynomial, ansatz wave function and 1/N expansion methods. The result for energy eigen value is also consistent to that obtained in this work.

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