Asymptotic iteration method for solution of the Kratzer potential in D-dimensional Klein-Gordon equation

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Abstract. The solution of D-dimensional Klein-Gordon equation for Kratzer potential was presented using asymptotic iteration method. The D-dimensional Klein-Gordon equation was reduced to one-dimensional radial differential equation. The Kratzer central potential was used in radial part solution to obtain the energy eigenvalues and radial wave function. The bound-state energy eigenvalues were calculated for various values of quantum numbers and dimensions using Matlab software.

1. Introduction

In many fields of physics, particularly quantum physics, atomic physics, and nuclear physics, for the relativistic case, Klein Gordon equation is the one of fundamental equation to describe the behavior of spinless microscopic particles. Solutions of Klein Gordon equation have been studied in many researches, both analytically and approximately. In earlier research, solution of Klein Gordon equation give the eigenvalue and eigen function which depend on the certainly potentials and certainly methods, such as Hulthen potential using Nikiforov–Uvarov [1], Hulthén-Type Potential using supersymmetric quantum mechanics (SUSYQM) [2], Makarov potential using factorization method [3], q-Deformed Manning-Rosen Potential using Asymptotic Iteration Method(AIM) [4], [5] and other. Recently, AIM has received much attention as a method for solving the Klein-Gordon equation [4], [6]–[8]. It has been applied to a large number of physically interesting potentials and has often yielded highly-accurate results.

The solution of Klein Gordon equation was mostly studied in three dimensional. But in recently, the solution of quantum system was extended in higher dimensions. Three dimensional space is embedded in a higher dimensional space. It was amazing that the force which influences until infinity range is so small compared to the electromagnetic force for example. Maybe we experience only a small part of it in our three dimensions and the major part is distributed to other dimensions we can’t perceive. So it is useful to deal with quantum mechanics in higher dimensions. The higher dimensions system in quantum physics has been studied in many cases, such as the solution of Klein-Gordon equation in D-dimensions for Hulthen potential [1], [2], Manning- Rosen potential [4], Kratzer potential [7], Morse potential [8], Poschl-Teller potential including centrifugal term [9], Hylleraas Potential [10], trigonometric Poschl-Teller potential [11], and other.

In this research, we investigated the Kratzer potential for D-dimensional Klein-Gordon using AIM. Kratzer potential is defined as [7], [12]

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\[ V(r) = -\frac{V_1}{r} + \frac{V_2}{r^2}, \quad S(r) = -\frac{S_1}{r} + \frac{S_2}{r^2} \]  
\[ (1) \]

The Klein-Gordon equation for Kratzer potential was reduced to Schrodinger like type equation, so it can be solved using AIM. AIM is one of alternative method. It has high efficiency and accuracy to determine eigen functions and eigen energies. [13]

2. Klein-Gordon Equation in D-dimensions

The time independent KG equation in D-dimensional with potentials of vector and scalar \( V(r) \) and \( S(r) \), respectively, with \( r = |\mathbf{r}| \) describing a spinless particle. In the general form the equation can write as [14]–[16]
\[ \nabla^2 D + \frac{1}{\hbar^2 c^2} \left[ (E - V(r))^2 - [Mc^2 + S(r)]^2 \right] \psi^{(l_{1,\ldots,l_{D-2}})}(x) = 0, \]  
\[ (2) \]

With \( E \) and \( M \) are the KG energy and the mass of particle. The \( x \) in equation (2) is a D-dimensional position vector. The laplacian \( \nabla^2 D \) is
\[ \nabla^2 D = \frac{1}{r^{D-1}} \frac{\partial}{\partial r} \left( r^{D-1} \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial \theta_{D-1}^2} + \frac{1}{r^2} \frac{\partial}{\partial \theta_{D-2}} \left( \sin \theta_{D-2} \sin \theta_{D-3} \cdots \sin \theta_{D-1} \right) \times \left\{ \frac{1}{\sin \theta_{D-1}} \frac{\partial}{\partial \theta_{D-1}} \sin \theta_{D-1} \frac{\partial}{\partial \theta_{D-1}} \right\} + \]  
\[ (3) \]

And
\[ \psi^{(l_{1,\ldots,l_{D-2}})}(x) = R_{l_{1,\ldots,l_{D-2}}}(r) Y^{(l)}(\theta_1, \theta_2, \ldots, \theta_{D-1}) \]  
\[ (4) \]

The wave function for radial part \( R_{l_{1,\ldots,l_{D-2}}}(r) \) is decomposed as
\[ R_{l_{1,\ldots,l_{D-2}}}(r) = r^{-l_{1,\ldots,l_{D-2}}/2} \tilde{F}(r), \]  
\[ (5) \]

If \( S = V \), it will produce a non-trivial nonrelativistic limit with a potential function \( 2V \) and not \( V \). Equation (2) is reduced to KG equation in D-dimension for radial part with the potential function \( V \) is scaled as \( 2V \). (in the relativistic atomic units \( \hbar = c = 1 \) [17]
\[ \nabla^2 D \psi^{(l_{1,\ldots,l_{D-2}})}(x) + [E^2 - M^2 - (E + M) V(r)] \psi^{(l_{1,\ldots,l_{D-2}})}(x) = 0, \]  
\[ (6) \]

3. Asymptotic Iteration Method (AIM)

AIM is used to solve the second order homogeneous equation of form [4], [6], [18], [19].
\[ y_n''(x) = \tilde{\lambda}_0(x) y_n'(x) + s_0(x) y_n(x) \]  
\[ (7) \]

with \( \tilde{\lambda}_0(x) \neq 0 \) and prime symbol denotes the derivative with respect to \( x \). The others parameter \( n \) is interpreted as the radial quantum number. The other variables, \( s_0(x) \) and \( \tilde{\lambda}_0(x) \) are differentiable.

To get the solution, we have to differentiate Eq. (7) along \( x \), and find
\[ y_n'''(x) = \tilde{\lambda}_1(x) y_n''(x) + s_1(x) y_n'(x) \]  
\[ (8) \]

Where
\[ \tilde{\lambda}_1(x) = \tilde{\lambda}_0'(x) + s_0(x) \tilde{\lambda}_0(x) \]  
\[ (9) \]
\[ s_1(x) = s_0'(x) + s_0(x) \tilde{\lambda}_0(x) \]  
\[ (10) \]

where \( \tilde{\lambda}_0(x) \neq 0 \) and \( s_0(x) \) is a function of \( C_\infty \) (coefficient of the differential equation) Asymptotic Iteration Method and can be applied exactly in the different problem if the wave function has been known and fulfill boundary condition zero (0) and infinity (\( \infty \)).

Equation (7) can be simple iterated until \( k+1 \) and \( k+2 \), \( k = 1, 2, 3, \ldots \) and then we get
\[ y_{n}^{k+1}(x) = \lambda_{k+1}(x) y_{n}^{k}(x) + s_{k+1}(x) y_{n}(x) \]  
(11)

\[ y_{n}^{k+2}(x) = \lambda_{k}(x) y_{n}^{k}(x) + s_{k}(x) y_{n}(x) \]  
(12)

where

\[ \lambda_{k}(x) = \lambda_{k+1}'(x) + s_{k+1}(x) + \lambda_{k}(x) \lambda_{k+1}(x) \]  
(13)

\[ s_{k}(x) = s_{k+1}'(x) + s_{0}(x) \lambda_{k+1}(x) \]  
(14)

Which is called recurrence relation. To determine the energy eigenvalues, we use quantization condition given by following equation

\[ \Delta_{k}(x) = \lambda_{k}(x) s_{k+1}(x) - \lambda_{k+1}(x) s_{k}(x) = 0 \]  
(15)

With the iteration number \( k \) is define as \( k = 1, 2, 3, \ldots \). The wave function can be determined using the wave function equation as follows

\[ y_{k}(x) = C_{2} \exp \left(-\int_{r}^{s_{k}} dx^* \right) \]  
(16)

4. Results and Discussion

Substituting equations (1, 2 – 5) into equation (6) we obtain

\[ \frac{1}{r^{D-1}} \frac{\partial}{\partial r} \left[ r^{D-1} \frac{\partial}{\partial r} F(r) \right] - \left[ (E + M \left( \frac{V_{1} + V_{2}}{r^{2}} \right)) + \left( E^{2} - M^{2} \left( \frac{F(r)}{r^{D-1/2}} + \left( E^{2} - M^{2} \right) \frac{F(r)}{r^{D-1/2}} \right) \right) = \lambda_{D-1} \frac{F(r)}{r^{D-1/2}} \]  
(17)

Where \( \lambda_{D-1} \) is the separation constant with \( \lambda_{D-1} = l(l + D - 2) \) and \( D \) is the dimension. Equation (17) can be simplify as

\[ \left[ \frac{d^{2}}{dr^{2}} - \frac{1}{r^{2}} \left( \left( \frac{D-1}{2} \right) \left( \frac{D-3}{2} \right) \right) - \lambda_{D-1} - (E + M V_{2}) \right] + \frac{1}{r} \left( E + M \right) V_{1} + \left( E^{2} - M^{2} \right) \right] F(r) = 0 \]  
(18)

By setting the part of equation (18),

\[ A(A+1) = \left( \frac{D-1}{2} \right) \left( \frac{D-3}{2} \right) - \lambda_{D-1} - (E + M V_{2}) \]  
(19)

\[ B = (E + M) V_{1} \]  
(20)

\[ E_{s}^{2} = (M^{2} - E^{2}) \]  
(21)

Then equation (18) become

\[ \frac{d^{2} F(r)}{dr^{2}} - \frac{A(A+1)}{r^{2}} F(r) + \frac{B}{r} F(r) - E_{s}^{2} F(r) = 0 \]  
(22)

By using Frobenius method, we let \( F(r) = r^{A} \sum C_{n} r^{n} \). The equation (22) has an irregular singularity \( r \to \infty \), where the normalized solution is \( F(r) \sim e^{-E_{s} r} \). When it has the singularity \( r \to 0 \), the \( F(r) \sim r^{A+1} \). To make equation (22) into form of equation (7), the wave function is set as follows

\[ F(r) = r^{A+1} e^{-E_{s} r} g(r) \]  
(23)

Substitute equation (23) into equation (22), we get

\[ g^\prime(r) = \left\{ 2E_{s} - \frac{2(A+1)}{r} \right\} g(r) + \left\{ \frac{2(A+1)E_{s} - B}{r} \right\} g(r) \]  
(24)

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Equation (24) is the homogeneous linear differential equation in second-order form. It can be solved by using AIM. By comparing equation (24) with equation (7), then we can get \( \lambda_0(r) \), and \( s_0(r) \). The \( \lambda_0(r) \), and \( s_0(r) \) can be calculated as follows

\[
\lambda_0 = \left\{ 2E_s - \frac{2(A+1)}{r} \right\},
\]

\[
s_0 = \left\{ \frac{2(A+1)E_s - B}{r} \right\}.
\]

\[
\lambda_1 = \frac{2(A+1)}{r^2} + \frac{2(A+1)E_s - B}{r} + \left( \frac{2E_s - \frac{2(A+1)}{r}}{r} \right)^2,
\]

\[
s_1 = -\frac{2(A+1)E_s - B}{r} + \frac{2(A+1)E_s - B}{r} \left( \frac{2E_s - \frac{2(A+1)}{r}}{r} \right), \text{ etc.}
\]

From equations (12–14, 25), we found the general eigenvalue of equation (24) in general term as follows

\[
E_{sn} = \frac{B}{2(A+1+n)}
\]

Where \( n \) is quantum number with \( n = 0,1,2,\ldots \). By substituting equation (19-21) to equation (26), the relativistic energy equation become

\[
M^2 - E_n^2 = \left[ \frac{(E_n + M)V_1}{2 \left\{ \sqrt{\left( \frac{D}{2} \right)\left( \frac{D-3}{2} \right) - \lambda_D - (E_n + M)V_2 + \frac{1}{4} + \frac{1}{2} + n} \right\} } \right]^2
\]

With \( V_1 \) and \( V_2 \) are the potential parameters where \( V_1 = 2D_ea \) and \( V_2 = D_ea^2 \). Where \( D_e \) and \( a \) are the dissociation energy and the equilibrium internuclear separation. For the Kratzer potential, when \( r \to 0 \) then the potential \( V(r) \to \infty \) because there is internuclear repulsion. When \( r \to \infty \) then the potential \( V(r) \to 0 \), i.e., the molecule decomposes [20].

Table 1. Various diatomic molecules reduced mass and spectroscopic properties in ground state.[20],[21]

| Parameter | CO | NO | O₂ | I₂ |
|-----------|----|----|----|----|
| \( D_e \) (eV) | 10.84514471 | 8.043782568 | 5.156658828 | 1.581791863 |
| \( a \) (Å) | 1.1282 | 1.1508 | 1.208 | 2.662 |
| \( M \) (amu) | 6.860586000 | 7.468441000 | 7.997457504 | 63.45223502 |

Table 1. presents the parameters for the potential. The potential parameter must be convert to natural unit where \( \hbar = c = 1 \). The \( a \) and \( M \) units are converted to \( 1/eV \) and \( eV \) due to the natural units. The relativistic energies value were calculated numerically from equation (27) by using Matlab. The results can be seen in Table 2.
Table 2. The relativistic energy $E_n$ in (GeV) with $l = 1$

| $D$ | $n$  | $CO$    | $NO$    | $O_2$    | $I_2$    |
|-----|------|---------|---------|---------|---------|
| 3   | 0    | -6.391161 | -6.957542 | -7.450621 | -59.106092 |
|     | 1    | -6.391725 | -6.958273 | -7.451656 | -59.106787 |
|     | 2    | -6.392854 | -6.959735 | -7.453726 | -59.108176 |
|     | 3    | -6.394546 | -6.961928 | -7.456831 | -59.110261 |
|     | 4    | -6.396803 | -6.964852 | -7.460970 | -59.113040 |
|     | 5    | -6.399623 | -6.968507 | -7.466145 | -59.116513 |
| 4   | 0    | -6.391020 | -6.957359 | -7.450363 | -59.105918 |
|     | 1    | -6.391584 | -6.958090 | -7.451397 | -59.106613 |
|     | 2    | -6.392713 | -6.959552 | -7.453467 | -59.108003 |
|     | 3    | -6.394405 | -6.961745 | -7.456572 | -59.110087 |
|     | 4    | -6.396662 | -6.964669 | -7.460712 | -59.112866 |
|     | 5    | -6.399482 | -6.968324 | -7.465886 | -59.116340 |
| 5   | 0    | -6.390597 | -6.956810 | -7.449586 | -59.105397 |
|     | 1    | -6.391161 | -6.957542 | -7.450621 | -59.106092 |
|     | 2    | -6.392289 | -6.959004 | -7.455796 | -59.107482 |
|     | 3    | -6.393982 | -6.961197 | -7.459935 | -59.109566 |
|     | 4    | -6.396238 | -6.964121 | -7.465110 | -59.112345 |
|     | 5    | -6.399059 | -6.967776 | -7.471319 | -59.115819 |

From Table 2., it is shown that the relativistic energy value is decreasing due to the increase of quantum number $n$. For higher dimension, the energy value is decreasing too. The relativistic energies for diatomic molecules of $CO$, $NO$, $O_2$, and $I_2$ are negative. The wave functions were determined using equation (16). And the graph of the wave function for $O_2$ particle are shown in Figure 1.
Figure 1. Four dimensional radial wave functions of $O_2$ with $l = 1$ (a) $n = 0$, (b) $n = 1$, and (c) $n = 2$. 
5. Conclusion
The bound-state energy eigenvalues of Klein-Gordon equation for Kratzer potential in D-dimension were obtained via asymptotic iteration method. From the results can be concluded that the relativistic energy value is decreasing due to the increase of quantum number \( n \). For higher dimension, the energy value is decreasing. The energy of diatomic molecules of \( CO \), \( NO \), \( O_2 \), and \( I_2 \) are negative.

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