Solution of three dimensional Schrodinger equation for Eckart and Manning-Rosen non-central potential using asymptotic iteration method

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Abstract. Solution of Schrodinger equation in three dimensions for Eckart and Manning-Rosen potential has been obtained by using the asymptotic iteration method. Energy spectrum and wave function for these potentials was obtained. It is known that the wave function for the corresponding potentials contains hypergeometric series due to the type of Schrodinger equation. However, the wave function for radial part is not normalizable, due to its equation that reaches to infinity when \( r \) equals to zero. The energy spectrum and wave function for corresponding potentials had also been analyzed with the help of Matlab R2013a software.

1. Introduction

Schrodinger equation is one of the most powerful tool to describe the phenomenon in quantum physics. One of its application is Coulomb potential, which is used to determine the probability of electron can be found in hydrogen atom. Nowadays, researchers had found many potentials that can describe the particular phenomena in the development of theoretical physics. These potentials are known as Poschl-Teller [1], Gendenshtein [2], Rosen-Morse [3], Eckart [4], Manning-Rosen potential [5], and so on.

Many researchers had studied the Schrodinger equation for these potentials. However, these potentials cannot be able to be solved exactly, so researchers studied these equations by using different approximation and methods. Here, we attempt to study the Schrodinger equation which is influenced by Eckart and Manning-Rosen potential, where Eckart potential as a radial function and Manning-Rosen as angular function. This is known as non-central potential.

Eckart potential is used to study the electron tunneling correction. Dong et al. [6], Falaye [7], and Resita [8] had studied Schrodinger equation for this potential in a different way, in particular, different variable substitution. In our work, we attempt to solve the Schrodinger equation with different variable substitution. Thus, in our work, there is Manning-Rosen potential which will determine the azimuthal and magnetic quantum number.

Our purpose of this work is to determine the energy spectrum and wave function of three dimensional Schrodinger equation for these potentials. To find the energy spectrum, we’re using the Asymptotic
**Iteration Method (AIM).** Researchers who had studied the Schrödinger equation used a variety of methods like Nikiforov-Uvarov (NU) [9], Romanovski polynomials [10], AIM [11], and so on. However, AIM is one of the most practical methods and often used by many researchers.

The approach of our work in order to solve the Schrödinger equation lies on variable substitution. Determined variable substitution may lead the equation to the type of hypergeometric equation. Our first “goal” is to find the hypergeometric type equation of corresponding Schrödinger equation before we treat the equation into AIM. Our hypergeometric type of equation is Gauss hypergeometric type equation. The other obtained Schrodinger equation will be treated similarly. The computer software that will be used to support this work will be MATLAB R2013a.

### 2. Overview of Asymptotic Iteration Method

Suppose we have the second order differential equation expressed as:

\[ y''_n = \lambda_0(x)y'_n + s_0(x)y_n \]  

If we differentiate Eq. (1) in respect to \( x \) in \( k \) times, Eq. (1) will become:

\[ y^{(k+2)}_n = \lambda_k(x)y'_n + s_k(x)y_n \]  

Where

\[ \lambda_k(x) = \lambda_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x) \]  

\[ s_k(x) = s_{k-1}(x) + s_0(x)\lambda_{k-1}(x) \]  

Next we’re going to examine the ratio between \( \lambda_k(x) \) and \( s_k(x) \). For a higher \( k \), it is found that

\[ \frac{\lambda_k(x)}{s_k(x)} = \alpha \]  

So that we’ll know the termination condition as

\[ \Delta = \lambda_k(x)s_{k-1}(x) - \lambda_{k-1}(x)s_k(x) = 0 \]  

This Eq. (6) will later be used to determine the energy spectrum and quantum numbers of the corresponding Schrodinger equation. For a complicated equation of \( \lambda_k(x) \) and \( s_k(x) \), calculation of Eq. (6) can be done easier with the help of computer.

### 3. Obtaining the Wave Function

In order to gain the wave function of the corresponding Schrodinger equation, we can use this second-order differential equation as reference.

\[ y''_n = 2\left(\frac{a^N}{(1-bz^{N+2})^2} - \frac{1}{z^2}\right)y'_n - \frac{wz^N}{(1-bz^{N+2})}y_n \]  

By transforming the Schrodinger equation to Eq. (7) form, we will be able to determine the parameters contained in Eq. (7) such as \( a, b, N \), and \( t \). The solution of Eq. (7) is expressed as

\[ y_n(x) = (-1)^nC_2(\sigma)_n(N + 2)^n\frac{\Gamma(-n, \rho + n; \sigma; b)z^{N+2}}{z^{(N+2)^2}} \]  

Where

\[ \rho = \frac{(2t+1)b+2a}{(N+2)b} \]  

\[ \sigma = \frac{N^2}{2t+1} \]  

\[ (\sigma)_n = \sigma(\sigma + 1)(\sigma + 2) \ldots (\sigma + n - 1) \]  

And \( C_2 \) is normalization constant. Parameter \((\sigma)_n\) in Eq. (11) is known as Pochhammer symbol, and have a similar expression as Pochhammer symbols contained in Eq. (12), which is known as Gauss hypergeometric series.

### 4. Three-Dimensional Schrodinger Equation for Eckart and Manning-Rosen Non-Central Potential

It is well-known that time-independent Schrödinger equation is expressed as follows

\[ \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + (E - V)\Psi(x) = 0 \]  

Where the potential we’re studying is non-central potential, expressed as
\[ V(r, \theta, \phi) = V(r) + \frac{V(\theta)}{r^2} + \frac{V(\phi)}{r^2 \sin^2 \theta} \]  

(14)

Here, the radial part of the non-central potential is Eckart potential, which is used to describe the electron penetration in potential barrier, or to describe the electron tunneling correction. The general Eckart potential is

\[ V(r) = -V_0 \frac{e^{-r/a}}{1 - e^{-r/a}} + V_1 \frac{e^{-r/a}}{(1 - e^{-r/a})^2} \]  

(15)

Where \( V_0 \) and \( V_1 \) are the depth of potential well and \( a \) is the length of potential. And trigonometric Manning-Rosen potential can be expressed as

\[ V(\theta) = \frac{V_2}{\sin^2 \theta} - V_3 \cot \theta \]  

(16)

And

\[ V(\phi) = \frac{V_4}{\cos^2 \phi} - V_5 \tan \phi \]  

(17)

Where the indexed variable \( V \) represents the depth of potential well, similar to Eq. (15). By substituting these potentials into Eq. (14) and (13), we obtain the Schrodinger equation for these potentials as

\[
\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \left[ E + V_0 \frac{e^{-r/a}}{1 - e^{-r/a}} - V_1 \frac{e^{-r/a}}{(1 - e^{-r/a})^2} - \frac{1}{r^2} \left( \frac{V_2}{\sin^2 \theta} - V_3 \cot \theta \right) - \frac{1}{r^2 \sin^2 \theta} \left( \frac{V_4}{\cos^2 \phi} - V_5 \tan \phi \right) \right] \Psi = 0
\]  

(18)

Using the parameter separation of \( \Psi(x) = R(r) r^{-1} P(\theta) H(\phi) \) and transforming the Schrodinger Equation into three dimension in spherical coordinate, we’ll be able to obtain three Schrodinger equation in radial, angular, and azimuthal part.

\[
\frac{\partial^2 R(r)}{\partial r^2} - \left[ \frac{2m}{\hbar^2} \left( -V_0 \frac{e^{-r/a}}{1 - e^{-r/a}} + V_1 \frac{e^{-r/a}}{(1 - e^{-r/a})^2} - E \right) - \frac{l'(l' + 1)}{r^2} \right] R(r) = 0
\]  

(19a)

\[
\frac{\partial^2 P(\theta)}{\partial \theta^2} + \cos \theta \frac{\partial P(\theta)}{\partial \theta} - \left[ \frac{2m}{\hbar^2} \left( \frac{V_2}{\sin^2 \theta} - V_3 \cot \theta \right) - \frac{m'^2}{\sin^2 \theta} - l'(l' + 1) \right] P(\theta) = 0
\]  

(19b)

\[
\frac{\partial H(\phi)}{\partial \phi} - \left[ \frac{2m}{\hbar^2} \left( \frac{V_4}{\cos^2 \phi} - V_5 \tan \phi \right) - m'^2 \right] H(\phi) = 0
\]  

(19c)

And the next step is to find the hypergeometric type of the corresponding Schrodinger equations, by using the variable and parameter substitution.

5. **Solving the Radial Part**

In Eq. (19a), if we substitute

\[ e^{-r/a} \approx -x \]  

(20)

Then using the approximation \( \frac{1}{r^2} \approx \frac{1}{a^2} (1 - e^{-r/a})^2 \) and substituting equations into Eq. (19a), we get

\[
\frac{\partial^2 R}{\partial x^2} + \frac{1 - 2x}{x(1-x)} \frac{\partial R}{\partial x} - \left[ \frac{(l'(l' + 1) - V_1 a^2)}{x(1-x)} - \frac{Ea^2}{x^2(1-x)} - \frac{Ea^2 - V_0 a^2}{x(1-x)} \right] R = 0
\]  

(21)

Equation (21) is the radial part of Schrodinger equation, which has a singular point at \( x = 0 \) and \( x = 1 \). By using series solution of \( R \)

\[ R = z^n \sum a_n z^n \]  

(22)

and substituting it into Eq. (21), we’re able to get the \( s \) parameter, and get the proportionality relation

\[ R \propto z^s \]  

(23)

based on Eq. (22). When \( x \to 0 \), the third term becomes a single term, instead of three terms as in Eq. (21), as its second term will become larger than the other term. Then Eq. (21) will become

\[
\frac{\partial^2 R}{\partial x^2} + \frac{1 - 2x}{x(1-x)} \frac{\partial R}{\partial x} + \frac{Ea^2}{x^2(1-x)} R = 0
\]  

(24)

Substituting \( R \) in Eq. (24) with Eq. (22), we’ll get the relation

\[ s^2 = \alpha^2 = -Ea^2 \]  

(25)

We can use the similar way for \( x \to 1 \) to obtain the different parameter \( s \). For this condition,

\[ s^2 = \beta^2 = -(Ea^2 - V_0 a^2) \]  

(26)
And from the proportionality relation in Eq. (23) for \( x \to 0 \) and \( x \to 1 \), we can obtain the wave equation in series form

\[
R = z^\alpha (1 - z)^\beta u(x)
\]

(27)

Where \( u(x) \) is a function. Then we can substitute Eq. (25), (26), and (27) into (21) in order to obtain the hypergeometric type Schrodinger equation. For the radial part, the hypergeometric type Schrodinger equation is written as

\[
x(1 - x) \frac{d^2u}{dx^2} + [(2\alpha + 1) - (2\alpha + 2\beta + 2)] \frac{du}{dx} - [(\alpha + \beta)(\alpha + \beta + 1) - (\ell'(\ell' + 1) - V_1a^2)]u = 0
\]

(28)

Where \( u \) is the function which contains hypergeometric series function. This function is similar to Eq. (8), and the parameters can be obtained by comparing the new Schrodinger equation with Eq. (7).

6. Solving the Angular and Azimuthal Part

We can use the same method as radial part to obtain the hypergeometric type Schrodinger equation for the angular and azimuthal part. For the angular part, we use the variable substitution as

\[
\cot \theta = i(1 - 2y)
\]

(29)

While for the azimuthal part is

\[
\tan \phi = i(1 - 2z)
\]

(30)

So we’re able to obtain the hypergeometric type Schrodinger equation for angular and azimuthal part

\[
y(1 - y) \frac{d^2v}{dy^2} + \left[(2\gamma + \frac{1}{2}) - (2\gamma + 2\delta + 1)\right] \frac{dv}{dy} - [(\gamma + \delta)^2 + (m'^2 - V_2)]v = 0
\]

(31)

\[
z(1 - z) \frac{d^2w}{dz^2} + [(2\zeta + 1) - (2\zeta + 2\eta + 2)] \frac{dw}{dz} - [(\zeta + \eta)(\zeta + \eta + 1) - V_4]w = 0
\]

(32)

Eq. (31) is for angular part, and (32) is azimuthal part, where the parameter substitution for angular part is written as

\[
-2\gamma(2\gamma - 1) = \ell'(\ell' + 1) - V_3i
\]

(33a)

\[
-2\delta(2\delta - 1) = \ell'(\ell' + 1) + V_3i
\]

(33b)

And for azimuthal part is

\[
-4\xi^2 = m'^2 - V_5i
\]

(34a)

\[
-4\eta^2 = m'^2 + V_5i
\]

(34b)

7. The Energy Spectrum

By using AIM we’re able to obtain the energy spectrum of Schrodinger equation for Eckart and Manning-Rosen Potential. From the three Schrodinger equations before, we know that the energy parameter is located in the radial part of Schrodinger equation. So, we’ll calculate the radial part of the hypergeometric type Schrodinger equation first using AIM. And the result of iteration is as follows:

\[
k = 0 \rightarrow c = (\alpha + \beta)(\alpha + \beta + 1)
\]

\[
k = 1 \rightarrow c = (\alpha + \beta + 1)(\alpha + \beta + 2)
\]

\[
k = 2 \rightarrow c = (\alpha + \beta + 2)(\alpha + \beta + 3)
\]

\[
k = 3 \rightarrow c = (\alpha + \beta + 3)(\alpha + \beta + 4)
\]

And so on, where \( c = (\ell'(\ell' + 1) - V_3a^2) \). So we’re able to obtain the pattern for this calculation

\[
c = (\alpha + \beta + n_r)(\alpha + \beta + n_r + 1)
\]

(35)

By substituting \( c, \alpha, \) and \( \beta \) from equations before, we’re able to obtain the energy spectrum for non-central Eckart and Manning-Rosen potential.

\[
E_{nl} = \frac{v_0}{2} - \frac{1}{a^2}\left[\frac{v_0^2a^4}{\sqrt{1+4\ell'(\ell'+1)-4V_1a^2(2n_r+1)}} + \frac{\sqrt{1+4\ell'(\ell'+1)-4V_1a^2(2n_r+1)}}{4}\right]
\]

(36)

Where \( \ell' \) is the orbital quantum number which depends on the Manning-Rosen potential. Table 1 shows the energy spectrum with the variation of \( n_r \) and \( \ell' \) when the particle isn’t influenced by Manning-Rosen potential, where \( a = V_0^{-1} \), \( V_0 = 0.005 \), and \( V_1 = 0.00005 \).
Table 1. The energy spectrum of a particle under the influence of Eckart potential with \( a = 1 / V_0 \), \( V_0 = 0.005 \), \( V_1 = 0.00005 \).

| No. | \( n_r \) | \( l \) | \( E_{nl} \)  |
|-----|-------|-----|----------|
| 1   | 1     | 0   | -0.00532 |
| 2   | 2     | 0   | -0.01519 |
| 3   | 2     | 1   | -0.06010 |
| 4   | 3     | 0   | -0.01116 |
| 5   | 3     | 1   | -0.02550 |

If the particle is influenced by Manning-Rosen potential, the \( \ell' \) parameter will depend on the potential depth of Manning-Rosen potential and quantum number \( n_c \). Note that \( \ell' \) will also depend on the magnetic quantum number \( m' \), while \( m' \) also depends on the potential depth of Manning-Rosen potential and quantum number \( n_m \). Both \( \ell' \) and \( m' \) can be determined by using AIM to the remaining Schrodinger equations, which are the angular and azimuthal part. Table 2 shows the energy spectrum of a particle under the influence of Eckart and Manning-Rosen potential.

Table 1. The energy spectrum of a particle under the influence of Eckart and Manning-Rosen potential with \( a = 1 / V_0 \), \( V_0 = 0.005 \), \( V_1 = 0.00005 \), \( V_2 = 10 \), \( V_3 = 5 \), \( V_4 = 80 \), \( V_5 = 150 \).

| No. | \( n_r \) | \( n_l \) | \( n_m \) | \( E \)   |
|-----|-------|-------|-------|--------|
| 1   | 1     | 0     | 0     | -0.12099 |
| 2   | 2     | 0     | 0     | -0.03609 |
| 3   | 2     | 1     | -1    | -0.04676 |
| 4   | 2     | 1     | 0     | -0.02406 |
| 5   | 2     | 1     | 1     | -0.01076 |

8. Wave Function

By comparing the hypergeometric type Schrodinger equation into Eq. (7), we’re able to obtain the wave function for corresponding Schrodinger equation. However, the obtained wave equations are not normalizable, due to the variable substitution, that cotangent and exponential terms diverge to infinity at \( \theta = 0 \) and \( r = 0 \), and the tangent term reaches infinity at \( \theta = \pi/2 \). Below is the graph of unnormalized wave function of radial part of Schrodinger equations for \( n_r = 2 \) and parameter values listed below.

Figure 1. Unnormalized radial part wave function of a particle influenced by Eckart and Manning-Rosen potential, where \( n_r = 2 \), \( n_l = 1 \), \( n_m = 0 \), \( a = 73.2 \), \( V_0 = 0.021 \), \( V_1 = 0.0021 \), \( V_2 = 0.5 \), \( V_3 = 0.1 \), \( V_4 = 1 \), \( V_5 = 0.1 \).
The wave function of radial part has decreasing amplitude, as $r$ goes higher. The curve is consistent for other value of $n$. However, the amplitude of wave function increases greatly in powers of ten as $n$ goes higher. The dead end at $r$ less than 0.002 denotes that as $r$ approach zero, the amplitude becomes negatively higher, and reaches minus infinity. For the angular and azimuthal part is shown in Figure 2.

![Figure 2](image)

**Figure 2.** (a) Unnormalized angular part wave function of a particle influenced by Eckart and Manning-Rosen potential, where $n_l = 1$, $n_m = 0$, $V_2 = 10$, $V_3 = 5$, $V_4 = 5$, $V_5 = 0.3$. (b) Unnormalized azimuthal part of wave function of a particle influenced by Eckart and Manning-Rosen potential, where $n_m = 1$, $V_4 = 5$, $V_5 = 0.3$.

However, these wave functions are solvable only for certain number of $n_l$ and $n_m$. The azimuthal part one doesn’t have a solution at $n_m$ higher than one.

9. **Conclusions**

In this paper, we’ve solved the three dimensional Schrödinger equation for Eckart and Manning-Rosen non-central potential using AIM. We’ve obtained the energy spectrum for particle which influenced by Eckart and Manning-Rosen potential for the certain value of quantum numbers. Also, we’ve obtained the unnormalized wave function of the particle which influenced by Eckart and Manning-Rosen potential, and visualize it into two-dimensional plot.

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11. **References**

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