N-Dimensional Solutions of Klein-Gordon Particles for Scaled Molecular Potential via Highly-Accurate Approximation

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ABSTRACT

The energy eigenvalues and eigenfunctions of relativistic scalar particles are obtained for an equal vector and scalar symmetrical molecular potential in N-dimensional euclidean space by using Asymptotic Iteration Method. For such a calculation, the potential in the eigenvalue equation is scaled regarding to fact that the potential is the same in non-relativistic limit. Furthermore, an highly-accurate approximation scheme is used to deal with the centrifugal term in the eigenvalue equation. The results obtained are compared with the ones that exist in literature.

Keywords: Klein-Gordon equation, Asymptotic Iteration Method, Symmetrical molecular potential, Centrifugal term

INTRODUCTION

Motion of scalar (i.e. spinless) particles in quantum mechanics is investigated by solving Klein-Gordon equation (relativistic case) or Schrödinger equation (non-relativistic case) for the interaction in system [1, 2]. This interaction is represented by a potential function which is crucial for solving the eigenvalue equation, since it acts a part to determine the solving technique.

The hyperbolic type molecular potential (or symmetrical well potential) [3] is one of the attractive potentials, and it represents some interactions in atomic and molecular levels. After Buyukkilic and friends introduced the potential and obtained one dimensional non-relativistic solutions in Ref.[3], many papers in which various solving methods are used, have been come out in the last decade. For instance, in Ref.[4], Yang has generalized the symmetrical well potential to the deformed one by way of the deformed hyperbolic functions [5]. In Ref.[6], exact solutions of relativistic cases have been obtained for l=0 states. Furthermore, Refs. [7, 8] can be added for using different solving methods to investigate the symmetrical well potential.

Recently, Candemir[9] has tackled Klein-Gordon equation in spherical-coordinates, for equal vector and scalar symmetrical well potential. She has obtained the solutions for states by using Nikiforov-Uvarov (NU) method[10]. She has also used Green-Aldrich approximation[11] to cope with the centrifugal term in the eigenvalue equation.

In this paper, the solutions of Klein-Gordon equation for equal vector and scalar symmetrical well potential is obtained in N-dimensional euclidean space. For the calculations, Asymptotic Iteration Method (AIM)[12, 13, 14] is used. Furthermore, an approximation scheme, which is more precise than Green-Aldrich approximation, is also used to eliminate the centrifugal term[15, 16]. Besides these, the potential is scaled considering that it should be the same in non-relativistic limit.

Organization of the paper is as follows: stationary Klein-Gordon equation for any equal vector and scalar potential is summarized in Section 2. Section 3 outlines AIM while it is used for obtaining the energy eigenvalues and eigenfunctions of Klein-Gordon equation for the symmetrical well potential in Section 4. The results are sums up in Section 5.

KLEIN-GORDON EQUATION FOR EQUAL VECTOR AND SCALAR POTENTIAL

Stationary (i.e. time-independent) Klein-Gordon equation for a potential that consists of vector and scalar components is given as follows ( \( \hbar = c = 1 \) )
\[
\left[ \nabla^2 + \left( V(\vec{r}) - \varepsilon \right)^2 - \left( S(\vec{r}) + m_0^2 \right)^2 \right] \psi(\vec{r}) = 0
\]  \hspace{1cm} (1)

where \( \varepsilon \) is relativistic energy, \( m_0 \) is rest mass, \( S(\vec{r}) \) and \( V(\vec{r}) \) are position-dependent scalar and vector potentials, respectively. In the case of \( S(\vec{r}) = \pm V(\vec{r}) \), Eq.(1) turns into

\[
\left[ \nabla^2 - 2\left( \varepsilon \pm m_0 \right)V(\vec{r}) + \varepsilon^2 - m_0^2 \right] \psi(\vec{r}) = 0
\]  \hspace{1cm} (2)

This equation is written in relativistic limit and, in general, stands for scalar particles. So, it is Klein-Gordon equation for the potential \( V(\vec{r}) \). Besides, it should give Schrödinger equation for the same potential in non-relativistic limit as mentioned by Alhaidari et al. in Ref.[17]. In case of \( S(\vec{r}) = +V(\vec{r}) \), non-relativistic limit of Eq.(2), in which \( \varepsilon - m_0 \approx E \) (E is non-relativistic energy and \( |E| = m_0 \) ), is yielded as

\[
\left[ \nabla^2 - 2V(\vec{r}) + E \right] \psi(\vec{r}) = 0
\]  \hspace{1cm} (3)

This is Schrödinger equation for the potential \( 2V(\vec{r}) \), not \( V(\vec{r}) \). Thus, one can scale the potentials in Eq.(1) as[17, 18]

\[
\left[ \nabla^2 + \left( \frac{1}{2} V(\vec{r}) - \varepsilon \right)^2 - \left( \frac{1}{2} S(\vec{r}) + m_0^2 \right)^2 \right] \psi(\vec{r}) = 0
\]  \hspace{1cm} (4)

As for the case of \( S(\vec{r}) = +V(\vec{r}) \), it can be written as

\[
\left[ \nabla^2 - \left( \varepsilon + m_0 \right)V(\vec{r}) + \varepsilon^2 - m_0^2 \right] \psi(\vec{r}) = 0
\]  \hspace{1cm} (5)

and this gives Schrödinger equation for the potential \( V(\vec{r}) \), in non-relativistic limit.

**A SUMMARY OF ASYMPTOTIC ITERATION METHOD (AIM)**

Asymptotic Iteration Method (AIM)[12] has been studied out as an alternative solution technique for, in general, second order linear differential equations given as

\[
f''(z) = \Lambda_0(z)f'(z) + \sigma_0(z)f(z)
\]  \hspace{1cm} (6)

where \( \Lambda_0(z) \) and \( \sigma_0(z) \) functions are in \( C^\infty \). The general solution of (6) is as follows (\( S_1 \) and \( S_2 \) are invariants)

\[
f(z) = \exp(-[\mu(t)dt] \times \left[ S_2 + S_1 \exp\left( \int\left( \Lambda_0(t) + 2\mu(t) dt \right) \right) \right]
\]  \hspace{1cm} (7)

in prospect of

\[
\frac{\sigma_n}{\sigma_{n-1}} = \frac{\Lambda_n}{\Lambda_{n-1}} = \mu
\]  \hspace{1cm} (8)

where \( n > 0 \) (\( n \in \mathbb{Z} \)) and

\[
\Lambda_n = \Lambda_{n-1} + \sigma_{n-1} + \Lambda_0 \Lambda_{n-1}, \quad \sigma_n = \sigma_{n-1} + \sigma_0 \Lambda_{n-1}
\]  \hspace{1cm} (9)

The functions \( \Lambda_0 \) and \( \sigma_0 \) contain the, \( E_n \), (unknown) energy eigenvalues when AIM is used in quantum mechanics in mathematical physics. These eigenvalues are obtained from the following equation

\[
\Delta_n(z,E) = \sigma_n(z,E)\Lambda_{n-1}(z,E) - \Lambda_n(z,E)\sigma_{n-1}(z,E) = 0
\]  \hspace{1cm} (10)

reached by the medium of Eq.(8). The eigenvalue problem is said to be "exactly solvable", if Eq.(10) depends upon only (unknown) \( E \) eigenvalues. In this case, an \( E_n \) energy eigenvalue is achieved after \( n \) iterations[19, 20, 21]. If Eq.(10) is also dependent on the variable \( z \), the energy eigenvalues are obtained approximately. Then, a suitable \( z = z_0 \) value should be determined for initiation of the AIM iterations[22, 23, 24].

As for obtaining the eigenfunctions of eigenvalue problem, following function generator is used in the view of AIM

\[
f_n(z) = S_2 \exp\left(-\int\frac{\sigma_n(t)}{\Lambda_n(t)} dt\right)
\]  \hspace{1cm} (11)

**THE SOLUTIONS OF KLEIN-GORDON EQUATION**

In this section, the eigenvalues and eigenfunctions of Klein-Gordon equation for the symmetrical well potential is obtained in N-dimensional euclidean space. For the calculations, AIM is used.
The stationary Klein-Gordon equation for equal scalar ($\mathcal{S}(\vec{r})$) and vector ($\mathcal{V}(\vec{r})$) potentials is given as in Eq.(5)

$$\left[\nabla^2 - (\varepsilon + m_0^2)\mathcal{V}(\vec{r}) + \varepsilon^2 - m_0^2\right] \psi(\vec{r}) = 0$$

For N-dimensional euclidean space, $\psi(\vec{r})$ is taken as

$$\psi(\vec{r}) = r^{\frac{N-1}{2}} u(r) Y_{l_1,l_2,...,l_{N-1}}(\phi_1,\phi_2,...,\phi_{N-1})$$

where $Y_{l_1,l_2,...,l_{N-1}}(\phi_1,\phi_2,...,\phi_{N-1})$ are hyperspherical harmonics and $l_1,l_2,...,l_{N-1}$ are angular momentum quantum numbers[25, 26, 27, 28, 29]. For spherical coordinates ($N = 3$), e.g., $l_{e_1} = m$ and $l_{e_2} = l$, while $\phi_{e_1}$ and $\phi_{e_2}$ are azimuthal and polar angles, respectively. Thus, for simpleness, the quantum number $l_{e_1}$ is abbreviated such as $l_{e_1} = l$ from now on.

Being $r \in (0, \infty)$, the radial Klein-Gordon equation in N-dimensions can be written as

$$\frac{d^2 u(r)}{dr^2} + \left[\frac{\varepsilon^2 - m_0^2}{r^2} - (\varepsilon + m_0) \mathcal{V}(r) - \frac{\gamma (\gamma + 1)}{r^2}\right] u(r) = 0$$

(13)

by using Eq.(12), where $\gamma = l + \frac{N-3}{2}$ and $\mathcal{V}(r)$ is the central potential of system.

As an attractive potential function, equal vector and scalar symmetrical well potential is given as

$$\mathcal{S}(\vec{r}) = \mathcal{V}(\vec{r}) = V_1 \left(\frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}\right)^2$$

$$+ V_2 \left(\frac{2}{e^{\alpha r} + e^{-\alpha r}}\right)^2$$

(14)

where $V_1$, $V_2$ and $\alpha$ are arbitrary constants. The form of the symmetrical well potential for a few $\alpha$ values can be seen in Fig.1.

For the potential in Eq.(14), Klein-Gordon equation which is given in Eq.(13) is written as

$$\frac{d^2 u(r)}{dr^2} + \left[\frac{\varepsilon^2 - m_0^2}{r^2} - (\varepsilon + m_0) V_1 \left(\frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}\right)^2$$

$$+ V_2 \left(\frac{2}{e^{\alpha r} + e^{-\alpha r}}\right)^2\right] u(r) = 0$$

In this equation an approximation scheme is used to deal with the $\gamma (\gamma + 1)/r^2$, centrifugal term. For this purpose, following approximation can be used [15]

$$\frac{1}{r} \approx 4\alpha^2 \left[C_0 + C_1 \left(\frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}\right)^2\right]$$

(16)

where the constants $C_0$ and $C_1$ are as follow

$$C_1 = \frac{\left(\frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}\right)^2}{4\alpha^2 \left(\frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}\right)^2}$$

As is seen in Fig. 2, the approximation in Eq.(16) is too close to the $1/r^2$ for either small or large values of the $\alpha$ [16].

Eq.(15) can be turned into the following equation by defining a new variable such as $x = \left(\frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}}\right)^2$ and using the approximation scheme given in Eq.(16)

$$\frac{d^2 u(x)}{dx^2} + \left(\frac{1}{2x} - \frac{1}{1-x}\right) \frac{du(x)}{dx}$$

$$+ \left(\frac{A}{x^2} + \frac{B}{(1-x)^2} + \frac{D}{x(1-x)}\right) u(x) = 0$$

(18)

where $x \in (0,1)$ and

$$A = -\kappa_1, \quad B = -\kappa_1 + \kappa_2 - \kappa_3, \quad D = -2\kappa_1 + \kappa_2$$

(19)

The constants $\kappa_1$, $\kappa_2$ and $\kappa_3$ are as below
The first-four iterations give the \( D \) as
\[
D_0 = \frac{1}{2}(7 + 5\beta + 6\rho + 4\beta\rho),
\]
\[
D_1 = \frac{1}{2}(18 + 9\beta + 10\rho + 4\beta\rho)
\]
\[
D_2 = \frac{1}{2}(33 + 13\beta + 14\rho + 4\beta\rho),
\]
\[
D_3 = \frac{1}{2}(52 + 17\beta + 18\rho + 4\beta\rho)
\]
So, one can generalize the \( D \) as below
\[
D_n = \frac{1}{2}\left[(2n^2 + 9n + 7) + (4n + 5)\beta + (4n + 6)\rho + 4\beta\rho\right] + (n - 1)\beta(\rho + 1) - D(\rho + 1)
\]
where \( n = 0, 1, 2, 3,... \)

Using Eqs.(25) and (26), the energy eigenvalues can be obtained analytically from the equation given below
\[
n(n + 1) + 2n\left[\sqrt{\frac{1}{16} + \kappa_1 + \kappa_3 - \kappa_2} - \frac{1}{4}\kappa_1 - \kappa_3 - \kappa_2 - 2\kappa_1 - \kappa_2 + \frac{1}{4}\right] = 0
\]
Some numeric values of the energy eigenvalues for $V_1 = 3$, $V_2 = 10$, $m_0 = 1$ and $\alpha = 0.125$ is given in Table 1.

Besides, comparison of the energy eigenvalues which have been calculated from Ref.[9] with the ones obtained for $N = 3$ dimensions in present study is given in Table 2.

As mentioned in Section 3, eigenfunctions of the problem is achieved through the function generator.

$$g_n(x) = \exp \left( \frac{-C_n(t)}{\Lambda_n(t)} \right)$$

function generator. For this purpose, functions in Eq.(24) are used.

Regarding to the first-four AIM iterations, outcomes given below are obtained for the function generator

$$g_0(x) = 1$$

$$g_1(x) = -(4\rho + 5) \left\{ 1 - \frac{[4(\beta + \rho) + 11]}{(4\rho + 5)} x^\beta \right\}$$

$$g_2(x) = (4\rho + 5) \times \left\{ 1 - \frac{2[4(\beta + \rho) + 13]}{(4\rho + 5)} x^\beta \right\}$$

$$g_3(x) = -(4\rho + 5)(4\rho + 7)(4\rho + 9) \times \left\{ 1 - \frac{3[4(\beta + \rho) + 15]}{(4\rho + 5)} x^\beta \right\}$$

If the following relation between Pochhammer symbol and $k$-Pochhammer symbol is used

$$\left( \frac{a}{k} \right)_n = k^d \left( \frac{a}{k} \right)_d$$

one can write the $g_n(x)$ as

$$g_{n,\beta,\rho}(x) = (-1)^n \left\{ \prod_{s=1}^{n} \left( 4\rho + 2s + 3 \right) \right\} \times \left\{ \sum_{\mu=0}^{n} \frac{(-n)\mu [4(\beta + \rho) + 2n + 9]_{\mu,2} x^\mu}{(4\rho + 5)_{\mu,2} \mu!} \right\}$$

where $n = 0, 1, 2, 3, \ldots$ and

$$(a)_d,k = a(a+k)(a+2k)(a+3k)\ldots(a+(d-1)k)$$

is $k$-Pochhammer symbol ($k \in \mathbb{R}$ and $d \in \mathbb{N}^+$) [30, 31].

### Table 1. Numeric values of the $E_n$ energy eigenvalues for $V_1 = 3$, $V_2 = 10$, $m_0 = 1$ and $\alpha = 0.125$, and for $N = 3, 6, 9$ dimensions. $E_n'$ represents the energy eigenvalues of antiparticle. The principle quantum number of an energy level is $(n+l+1)$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Energy level</th>
<th>$E_n$</th>
<th>$E_n'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1s</td>
<td>-0.982158</td>
<td>-0.999150</td>
</tr>
<tr>
<td>2s</td>
<td>-0.901930</td>
<td>-0.994573</td>
<td></td>
</tr>
<tr>
<td>2p</td>
<td>-0.946310</td>
<td>-0.998056</td>
<td></td>
</tr>
<tr>
<td>4p</td>
<td>-0.680055</td>
<td>-0.981598</td>
<td></td>
</tr>
<tr>
<td>4d</td>
<td>-0.757918</td>
<td>-0.988561</td>
<td></td>
</tr>
<tr>
<td>5d</td>
<td>-0.581474</td>
<td>-0.976690</td>
<td></td>
</tr>
<tr>
<td>6d</td>
<td>-0.375575</td>
<td>-0.961079</td>
<td></td>
</tr>
<tr>
<td>6f</td>
<td>-0.473204</td>
<td>-0.971551</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1s</td>
<td>-0.921555</td>
<td>-0.997383</td>
</tr>
<tr>
<td>2s</td>
<td>-0.799418</td>
<td>-0.990154</td>
<td></td>
</tr>
<tr>
<td>2p</td>
<td>-0.859335</td>
<td>-0.995781</td>
<td></td>
</tr>
<tr>
<td>4p</td>
<td>-0.528440</td>
<td>-0.974152</td>
<td></td>
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<tr>
<td>4d</td>
<td>-0.614897</td>
<td>-0.983550</td>
<td></td>
</tr>
<tr>
<td>5d</td>
<td>-0.415974</td>
<td>-0.968884</td>
<td></td>
</tr>
<tr>
<td>6d</td>
<td>-0.195785</td>
<td>-0.950587</td>
<td></td>
</tr>
<tr>
<td>6f</td>
<td>-0.296301</td>
<td>-0.963340</td>
<td></td>
</tr>
</tbody>
</table>
So, the unnormalized $u_n(x)$, given in Eq.(21), is got as follows

$$u_n(x) = (-1)^n \xi_n x^\frac{1}{4} \frac{1}{\sqrt{16 \kappa_1}} (1-x)^\frac{\kappa_1 + \kappa_2}{3} \prod_{\kappa=1}^{\kappa_n} (4\rho + 2s + 3)$$ \hspace{1cm} (31)

where $\xi_n$ is normalization constant, and $\rho$ and $\beta$ is given as Eq.(23).

Table 2. Comparison of the $E_n^r$ energy eigenvalues calculated from Ref.[9] with the ones of present study in spherical coordinates ($N=3$) for $V_1 = 3$, $V_2 = 10$, $m_0 = 1$ and $\alpha = 0.125$. $E_n^r$ represents the antiparticle's energy.

<table>
<thead>
<tr>
<th>Energy level</th>
<th>$E_n$</th>
<th>$E_n$ from Ref.[9]</th>
<th>$E_n^r$</th>
<th>$E_n^r$ from Ref.[9]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>-0.982158</td>
<td>-0.993527</td>
<td>-0.999150</td>
<td>-0.999535</td>
</tr>
<tr>
<td>2s</td>
<td>-0.901930</td>
<td>-0.963422</td>
<td>-0.994573</td>
<td>-0.997050</td>
</tr>
<tr>
<td>2p</td>
<td>-0.946310</td>
<td>-0.981451</td>
<td>-0.998056</td>
<td>-0.998542</td>
</tr>
<tr>
<td>4p</td>
<td>-0.680055</td>
<td>-0.874758</td>
<td>-0.981598</td>
<td>-0.989587</td>
</tr>
<tr>
<td>4d</td>
<td>-0.757918</td>
<td>-0.909933</td>
<td>-0.988561</td>
<td>-0.992573</td>
</tr>
<tr>
<td>5d</td>
<td>-0.581474</td>
<td>-0.834196</td>
<td>-0.976690</td>
<td>-0.986102</td>
</tr>
<tr>
<td>6d</td>
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<td>-0.737735</td>
<td>-0.961079</td>
<td>-0.977635</td>
</tr>
<tr>
<td>6f</td>
<td>-0.473204</td>
<td>-0.788449</td>
<td>-0.971551</td>
<td>-0.982119</td>
</tr>
</tbody>
</table>

**CONCLUSION**

In quantum mechanics, a physical system undergoes a potential is investigated by obtaining the energy eigenvalues and eigenfunctions. This goal is achieved via several mathematical methods. Asymptotic Iteration Method (AIM)[12] is one of the methods widely used. It has some advantages such that it can be applied to both exactly and approximately (numerically) solvable problems. It is also used to obtain perturbative energy eigenvalues calculated from Ref.[9]. It has been seen that the energy eigenvalues are greater than those of Ref.[9] in which calculations have been made in spherical coordinates and Green-Aldrich approximation[11] has been used to eliminate the centrifugal term (see in Table 2). This difference becomes more clear especially for higher quantum levels. One reason for such a conclusion can be resulted from that the eigenvalues have been obtained for the symmetrical well potential, let’s say $V(r)$, in present study whereas the eigenvalues have been resulted for $V(r)$ in Ref.[9]. So, in present study, it is more likely to be free-particle system.

Besides, accuracy of the approximation scheme used can be illuminated by Eq.(17) (also seen in Fig.2). According to this equation, $C_0$ and $C_1$ constants are also dependent upon the $\alpha$ arbitrary parameter. So, they correspondingly change in any variation of $\alpha$.

**REFERENCES**