

# 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.

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## 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 adduced 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  $l=0$  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 ( $\hbar = c = 1$ )

$$\left[ \bar{\nabla}^2 + (V(\vec{r}) - \varepsilon)^2 - (S(\vec{r}) + m_0)^2 \right] \psi(\vec{r}) = 0 \quad (1)$$

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

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

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  $|E| \approx m_0$ ), is yielded as

$$\left[ \frac{\nabla^2}{2m_0} - 2V(\vec{r}) + E \right] \psi(\vec{r}) = 0 \quad (3)$$

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]

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

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

$$\left[ \bar{\nabla}^2 - (\varepsilon + m_0)V(\vec{r}) + \varepsilon^2 - m_0^2 \right] \psi(\vec{r}) = 0 \quad (5)$$

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

$$f''(z) = \Lambda_0(z)f'(z) + \sigma_0(z)f(z) \quad (6)$$

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)

$$f(z) = \exp(-\int \mu(t) dt) \times \left[ S_2 + S_1 \int \exp\left(\int (\Lambda_0(\tau) + 2\mu(\tau)) d\tau\right) dt \right] \quad (7)$$

in prospect of

$$\frac{\sigma_n}{\sigma_{n-1}} = \frac{\Lambda_n}{\Lambda_{n-1}} \equiv \mu \quad (8)$$

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

$$\Lambda_n = \Lambda'_{n-1} + \sigma_{n-1} + \Lambda_0 \Lambda_{n-1}, \quad \sigma_n = \sigma'_{n-1} + \sigma_0 \Lambda_{n-1} \quad (9)$$

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

$$\Lambda_n(z, E) \equiv \sigma_n(z, E) \Lambda_{n-1}(z, E) - \Lambda_n(z, E) \sigma_{n-1}(z, E) = 0 \quad (10)$$

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  $z \approx z_0$  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

$$f_n(z) = S_2 \exp\left(-\int \frac{\sigma_n(t)}{\Lambda_n(t)} dt\right) \quad (11)$$

## 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 ( $S(\vec{r})$ ) and vector ( $V(\vec{r})$ ) potentials is given as in Eq.(5)

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

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

$$\psi(\vec{r}) = r^{-\frac{(N-1)}{2}} u(r) Y_{l_1, l_2, \dots, l_{N-1}}(\varphi_1, \varphi_2, \dots, \varphi_{N-1}) \quad (12)$$

where  $Y_{l_1, l_2, \dots, l_{N-1}}(\varphi_1, \varphi_2, \dots, \varphi_{N-1})$  are hyperspherical harmonics and  $l_1, l_2, \dots, l_{N-1}$  are angular momentum quantum numbers [25, 26, 27, 28, 29]. For spherical coordinates ( $N = 3$ ), e.g.,  $l_{N-2} \equiv m$  and  $l_{N-1} \equiv l$ , while  $\varphi_{N-2}$  and  $\varphi_{N-1}$  are azimuthal and polar angles, respectively. Thus, for simpleness, the quantum number  $l_{N-1}$  is abbreviated such as  $l_{N-1} \equiv l$  from now on.

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

$$\frac{d^2 u(r)}{dr^2} + \left[ (\varepsilon^2 - m_0^2) - (\varepsilon + m_0)V(r) - \frac{\gamma(\gamma+1)}{r^2} \right] u(r) = 0 \quad (13)$$

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

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

$$S(r) = V(r) = V_1 \left( \frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}} \right)^2 + V_2 \left( \frac{2}{e^{\alpha r} + e^{-\alpha r}} \right)^2 \quad (14)$$

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

$$\frac{d^2 u(r)}{dr^2} + \left\{ \begin{aligned} & \left( \varepsilon^2 - m_0^2 \right) - (\varepsilon + m_0) \times \\ & \left[ V_1 \left( \frac{e^{\alpha r} - e^{-\alpha r}}{e^{\alpha r} + e^{-\alpha r}} \right)^2 + \right. \\ & \left. V_2 \left( \frac{2}{e^{\alpha r} + e^{-\alpha r}} \right)^2 \right] \\ & - \frac{\gamma(\gamma+1)}{r^2} \end{aligned} \right\} u(r) = 0$$

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]

$$\frac{1}{r^2} \approx 4\alpha^2 \left[ C_0 + C_1 \left( \frac{e^{\alpha r}}{e^{2\alpha r} - 1} \right)^2 \right] \quad (16)$$

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

$$C_1 = \frac{(e^{2\alpha} - 1)^3}{4\alpha^3 e^{2\alpha} (e^{2\alpha} + 1)}, \quad C_0 = \frac{1}{4\alpha^2} - C_1 \frac{e^{2\alpha}}{(e^{2\alpha} - 1)^2} \quad (17)$$

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)

$$\frac{d^2 u(x)}{dx^2} + \left( \frac{1}{2x} - \frac{1}{1-x} \right) \frac{du(x)}{dx} + \left( \frac{A}{x^2} + \frac{B}{(1-x)^2} + \frac{D}{x(1-x)} \right) u(x) = 0 \quad (18)$$

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

$$A = -\kappa_1, \quad B = -\kappa_1 + \kappa_2 - \kappa_3, \quad D = -2\kappa_1 + \kappa_2 \quad (19)$$

The constants  $\kappa_1$ ,  $\kappa_2$  and  $\kappa_3$  are as below

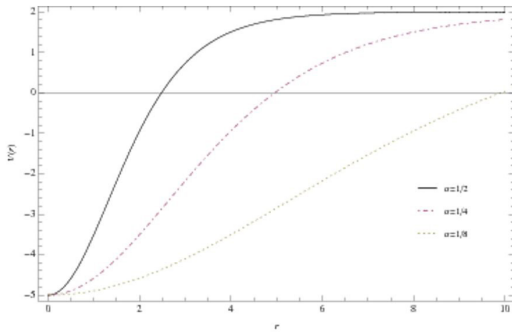


Figure 1. Shape of the symmetrical well potential for  $V_1 = 2$ ,  $V_2 = 5$ , and  $\alpha = 0.5, 0.25, 0.125$ . The  $\alpha$  determines the range of the potential well and  $V_1, V_2$  specify the well depth

$$\begin{aligned} \kappa_1 &= C_1 \frac{\gamma(\gamma+1)}{4} \\ \kappa_2 &= -C_0 \gamma(\gamma+1) + C_1 \frac{\gamma(\gamma+1)}{4} + \frac{(\varepsilon + m_0)}{4\alpha^2} V_2 \\ &\quad + \frac{(\varepsilon^2 - m_0^2)}{4\alpha^2} \\ \kappa_3 &= \frac{(\varepsilon + m_0)}{4\alpha^2} (V_1 + V_2) \end{aligned} \quad (20)$$

Regarding to the boundary conditions of the system, one can assume (unnormalized)  $u(x)$  in Eq.(18) as follows

$$u(x) = x^{\frac{1}{4}} + \sqrt{\frac{1}{16} + \kappa_1} (1-x) \sqrt{\kappa_1 + \kappa_3 - \kappa_2} g(x) \quad (21)$$

where  $g(x)$  is the function to be determined by AIM. If  $u(x)$ , given by Eq.(21), is substituted in Eq.(18) following equation is obtained

$$\begin{aligned} \frac{d^2 g(x)}{dx^2} + \left[ \frac{\left(2\rho + \frac{5}{2}\right)}{x} - \frac{(2\beta + 3)}{1-x} \right] \frac{dg(x)}{dx} \\ - \left[ \frac{\left(2\rho + \frac{5}{2}\right)(\beta + 1)}{x(1-x)} - \frac{D - (\rho + 1)}{x(1-x)} \right] g(x) = 0 \end{aligned} \quad (22)$$

where

$$\rho = -\frac{3}{4} + \sqrt{\frac{1}{16} + \kappa_1}, \quad \beta = -1 - \sqrt{\kappa_1 + \kappa_3 - \kappa_2}$$

Eq.(22) is in AIM form, and the iterations can be initiated using the following functions, in keeping with Eq.(6)

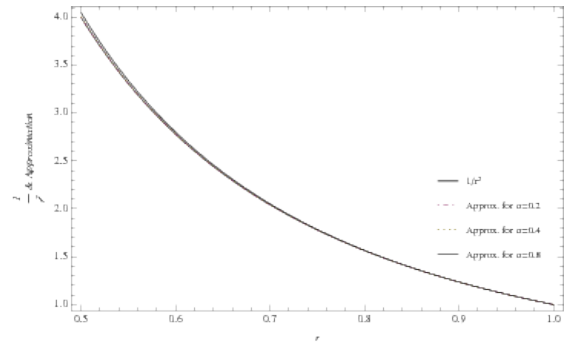


Figure 2. Comparison of the  $1/r^2$  centrifugal term and the approximation scheme. The approximation is too close to (even overlapped) the centrifugal term for either small or large values of the  $\alpha$

$$\begin{aligned} \Lambda_0(x) &= - \left[ \frac{\left(2\rho + \frac{5}{2}\right)}{x} - \frac{(2\beta + 3)}{1-x} \right], \\ \sigma_0(x) &= \left[ \frac{\left(2\rho + \frac{5}{2}\right)(\beta + 1)}{x(1-x)} - \frac{D - (\rho + 1)}{x(1-x)} \right] \end{aligned} \quad (24)$$

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

$$D_n = \frac{1}{2} \left[ \frac{(2n^2 + 9n + 7) + (4n + 5)\beta}{+(4n + 6)\rho + 4\beta\rho} \right] \quad (25)$$

where  $n = 0, 1, 2, 3, \dots$

Using Eqs.(25) and (??), the energy eigenvalues can be obtained analytically from the equation given below

$$\begin{aligned} n(n+1) + 2n \left( \sqrt{\frac{1}{16} + \kappa_1} - \sqrt{\kappa_1 + \kappa_3 - \kappa_2} \right) \\ - 2 \sqrt{\frac{1}{16} + \kappa_1} (\kappa_1 + \kappa_3 - \kappa_2) \\ + \sqrt{\frac{1}{16} + \kappa_1} - \sqrt{\kappa_1 + \kappa_3 - \kappa_2} + 2\kappa_1 - \kappa_2 + \frac{1}{4} = 0 \end{aligned} \quad (26)$$

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,  $g_n(x) = \exp\left(-\int \frac{\sigma_n(t)}{\Lambda_n(t)} dt\right)$ , function generator. For this purpose, and functions in Eq.(24) are used.

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

$$g_0(x) = 1$$

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

$$g_2(x) = (4\rho+5) \times \left\{ \begin{aligned} &1 - \frac{2[4(\beta+\rho)+13]}{(4\rho+5)} x \\ &+ \frac{2[4(\beta+\rho)+13][4(\beta+\rho)+15]}{(4\rho+5)(4\rho+7)} x^2 \end{aligned} \right\} \times \frac{1}{2!}$$

$$g_3(x) = -(4\rho+5)(4\rho+7)(4\rho+9)$$

$$\times \left\{ \begin{aligned} &1 - \frac{3[4(\beta+\rho)+15]}{(4\rho+5)} x \\ &+ \frac{6[4(\beta+\rho)+15][4(\beta+\rho)+17]}{(4\rho+5)(4\rho+7)} x^2 \\ &- \frac{6[4(\beta+\rho)+15][4(\beta+\rho)+17][4(\beta+\rho)+19]}{(4\rho+5)(4\rho+7)(4\rho+9)} x^3 \end{aligned} \right\} \times \frac{1}{3!}$$

Accordingly, the  $g_n(x)$  function generator can be obtained as

$$g_{n,\beta,\rho}(x) = (-1)^n \left\{ \prod_{s=1}^n (4\rho+2s+3) \right\} \times \left\{ \sum_{\mu=0}^n \frac{(-n)_\mu [4(\beta+\rho)+2n+9]_{\mu,2} x^\mu}{(4\rho+5)_{\mu,2} \mu!} \right\} \quad (27)$$

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

$$(a)_{d,k} = a(a+k)(a+2k)(a+3k)\dots(a+(d-1)k) \quad (28)$$

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

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

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  $(n+l+1)$ .

N	Energy level	$E_n$	$E'_n$
3	1s	-0.982158	-0.999150
	2s	-0.901930	-0.994573
	2p	-0.946310	-0.998056
	4p	-0.680055	-0.981598
	4d	-0.757918	-0.988561
	5d	-0.581474	-0.976690
6	6d	-0.375575	-0.961079
	6f	-0.473204	-0.971551
	1s	-0.921555	-0.997383
	2s	-0.799418	-0.990154
	2p	-0.859335	-0.995781
	4p	-0.528440	-0.974152
9	4d	-0.614897	-0.983350
	5d	-0.415974	-0.968884
	6d	-0.195785	-0.950587
	6f	-0.296301	-0.963340
	1s	-0.822311	-0.994852
	2s	-0.665414	-0.985163
9	2p	-0.737623	-0.992735
	4p	-0.356946	-0.966148
	4d	-0.449066	-0.977435
	5d	-0.234210	-0.960458
	6d	-0.004814	-0.939539
	6f	-0.106303	-0.954464

$$(a)_{d,k} = k^d \left(\frac{a}{k}\right)_d \quad (29)$$

one can write the  $g_n(x)$  as

$$g_{n,\beta,\rho}(x) = (-1)^n \left\{ \prod_{s=1}^n (4\rho+2s+3) \right\} \times {}_2F_1\left(-n, \frac{4(\beta+\rho)+2n+9}{2}; \frac{4\rho+5}{2}; x\right) \quad (30)$$

where  ${}_2F_1(a,b;c;x)$  is the hypergeometric function.

So, the unnormalized  $u_n(x)$ , given in Eq.(21), is got as follows

$$u_n(x) = (-1)^n \xi_n x^{\frac{1}{4} + \sqrt{\frac{1}{16} + \kappa_1}} (1-x)^{\sqrt{\kappa_1 + \kappa_3 - \kappa_2}} \left\{ \prod_{s=1}^n (4\rho + 2s + 3) \right\} \quad (31)$$

$$\times {}_2F_1\left(-n, \frac{4(\beta + \rho) + 2n + 9}{2}; \frac{4\rho + 5}{2}; x\right)$$

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

Table 2. Comparison of the  $E_n$  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  $\alpha = 0.125$   $E'_n$  represents the antiparticle's energy.

Energy level	$E_n$	$E_n$ from Ref.[9]	$E'_n$	$E'_n$ from Ref.[9]
1s	-0.982158	-0.993527	-0.999150	-0.999535
2s	-0.901930	-0.963422	-0.994573	-0.997050
2p	-0.946310	-0.981451	-0.998056	-0.998542
4p	-0.680055	-0.874758	-0.981598	-0.989587
4d	-0.757918	-0.909933	-0.988561	-0.992573
5d	-0.581474	-0.834196	-0.976690	-0.986102
6d	-0.375575	-0.737735	-0.961079	-0.977635
6f	-0.473204	-0.788449	-0.971551	-0.982119

## CONCLUSION

In quantum mechanics, a physical system undergone 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 eigenvalues and eigenfunctions besides the non-perturbative usage[13, 32, 33].

In present study, a system which is under the influence of a hyperbolic type molecular potential (or symmetrical well potential)[3] is probed. By using this potential, one can obtain the reflectionless potential and a particular case of hyperbolic type molecular potential which has a relation with three-dimensional harmonic oscillator [9, 34, 35]. The eigenvalues and eigenfunctions of Klein-Gordon equation

have been obtained using AIM. Results have been obtained for  $d$ -dimensional euclidean space. An highly-accurate approximation scheme[15, 16] has been also used to deal with the centrifugal term. Furthermore, potential term in the Klein-Gordon equation has been scaled taking the consideration that the potential should be the same in non-relativistic limit, i.e. Schrödinger equation[17, 18]. For the calculations, the case of equal vector and scalar symmetrical well potential has been considered.

The results achieved have also been compared with the ones 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 the  $\alpha$ .

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