
Araştırma Makalesi / Research Article

An Analytical Expression for The Eigenvalues of The Potential Family

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

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Abstract

In the current study, we introduce an analytical form of the solution for the potential family $V(r) = \frac{A}{r^2} - \frac{B}{r} + Cr^\kappa$. The method which combines the perturbation theory (PT) and supersymmetric (SUSY) quantum theory results in an abstract equation of the energy eigenvalues (which can be named as closed analytical form method (CAFMM)). The results of the asymptotic iteration method (AIM) and CAFMM will be compared with the numerical method (NM) to test the validity of our approximation at the end of the work.

Keywords: Solutions of wave equations: bound states, Supersymmetry, Algebraic methods.

$$V(r) = \frac{A}{r^2} - \frac{B}{r} + Cr^\kappa \text{ Potansiyel Ailesinin Özdeğerlerini Veren Analitik İfade}$$

Öz

Bu çalışmada, $V(r) = \frac{A}{r^2} - \frac{B}{r} + Cr^\kappa$ potansiyel ailesine ait çözümleri veren analitik bir ifade önerdik. Süpresimetrik kuantum teorisi ile pertürbasyon teorisini birleştiren bu metod enerji özdeğerlerini içeren bir denklem sağlamaktadır (metod kapalı analitik form olarak adlandırılabilir). Çalışmanın sonunda yaklaşımımızın geçerliliğini tespit etmek için, asimptotik iterasyon metodu ve kapalı analitik form metoduna ait sonuçlar nümerik metotla karşılaştırılacaktır.

Anahtar kelimeler: Dalga denklemleri çözümleri: bağlı durum, Süpresimetri, Cebirsel metotlar.

1. Introduction

In quantum mechanics, the successful description of a system formed by interacting particles can be achieved by using a convenient potential endowed with suitable parameters. Some numerical approaches or approximation techniques for solving the Schrödinger equation for non-solvable potentials play an important role to investigate the ground and excited electronic states of the quantum system. As well known, an exact analytical solution has been achieved for limited potentials. Coulomb and Harmonic oscillator potentials are two important examples of the solvable potentials [1]. The potentials such as Yukawa [2] and Woods-Saxon [3] have been numerically solved or analyzed by using some approximation techniques giving numerical eigenvalues and eigenfunction.

In our previous study, we have treated the Gaussian-type potential aiming to form a closed analytical equation of the corresponding eigenvalues [4]. In this work, we have followed a technique which was used to solve the Yukawa-type potentials. And we obtained a closed-form of eigenvalue equation for a single particle in Gaussian potential.

In current work, we are analyzing a potential family $V(r) = \frac{A}{r^2} - \frac{B}{r} + Cr^\kappa$ [5] of which importance is the result of the possibility to transform it into the different type of potentials by varying

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the parameters A , B and C . Aygun et. al. [5] reported that some cases of this potential family can be solved analytically and numerical treatment has been required to solve other cases.

Here, we concentrate on derivation of an analytical expression for the eigenvalues of a single particle in this potential family. For this purpose, we try to combine the perturbation theory and supersymmetric quantum theory following the treatment [6] performed in our previous study.

In the next section we present the theory and formalism. Section 3 provides the results. Section 4 is devoted to our conclusions.

2. Theory and Formalism

In the study, we investigate the potential family

$$V(r) = \frac{A}{r^2} - \frac{B}{r} + Cr^\kappa \tag{1}$$

where A , B and C and κ are the parameters which modify the potential terms. One should notice that for some special values of the parameters will give solvable potentials. For example, in the case of $A = C = 0$ the potential turns into the Coulomb whereas the case of $A = B = 0$ and $\kappa = 2$ transforms the potential into the Harmonic Oscillator.

2.1. Closed-Analytical-Form Method (CAFEM)

In principle, all the potentials can be considered as a different version of another one. The potential family in Eq. (1) can be assumed as the expansion of an exponential potential which reads

$$V(r) = -B \frac{e^{-\alpha r^{\kappa+1}}}{r} \tag{2}$$

In the case of Taylor expansion, it will be

$$V(r) = -\frac{B}{r} + B\alpha r^\kappa - \frac{\alpha^2 B r^{2\kappa-1}}{2!} + \frac{\alpha^3 B r^{3\kappa-1}}{3!} - \dots \tag{3}$$

where the parameter α should be considered as small value. The Coulomb potential term can be treated as an unperturbed part of Eq. (3).

The term or A/r^2 or C/r^2 in the case of $\kappa = -2$ are the expressions which are very similar to the barrier term $\hbar^2 \ell(\ell + 1)/2mr^2$. Because of the small value of α , the contribution of $C = B\alpha$ and other expansion terms can be simply ignored. In that case, the summation of these three terms will be equal to the barrier term $\hbar^2 \ell'(\ell' + 1)/2mr^2$. In the case of $\kappa = -1$, the C/r term can be considered as a parameter in the Coulomb potential. In the case of $\kappa = 0$, the last term only provides additional energy.

Unfortunately, this method can not approximate the energy values in the case of $\kappa < -2$. Here, as a method, we assume that potential family is a kind of expansion of an exponential potential (as in the case of Gaussian or Yukawa potentials).

As well known from the literature, the normalized wave the function of the Coulomb potential is

$$\begin{aligned} \chi_{n\ell'} = & \left(\frac{2mB}{(n + \ell' + 1)\hbar^2} \right)^{\ell'+1} \times \frac{r^{\ell'+1}}{(n + \ell' + 1)\sqrt{\hbar(n + 2\ell' + 1)!/(mBn!)}} \\ & \times e^{-\frac{mB}{(n+\ell'+1)\hbar^2 r}} L_n^{2\ell'+1} \left(\frac{2Bmr}{\hbar^2(n + 2\ell' + 1)} \right) \end{aligned} \tag{4}$$

where m and \hbar are electron mass and Planck's constant, respectively and $L_n^{2\ell'+1} \left(\frac{2Bmr}{\hbar^2(n+2\ell'+1)} \right)$ is Associated Laguerre polynomial. Here, the corresponding eigenvalue of the Coulomb potential term can be written as

$$E_{n,\ell'} = -\frac{mB^2}{2\hbar^2(n + \ell' + 1)^2} \tag{5}$$

Perturbative wavefunctions, energies and superpotentials corresponding to the modification potentials are

$$\begin{aligned} \Delta V(r; \epsilon) &= \sum_{k=1}^{\infty} \epsilon^k \Delta V^{\{k\}}(r) \\ \Delta W_{n\ell'}(r; \epsilon) &= \sum_{k=1}^{\infty} \epsilon^k \Delta W_{n\ell'}^{\{k\}}(r) \\ \Delta E_{n\ell'}(r; \epsilon) &= \sum_{k=1}^{\infty} \epsilon^k \Delta E_{n\ell'}^{\{k\}} \end{aligned} \tag{6}$$

where k indicates the perturbation order. If the unknown perturbed wavefunction is $R_p(r)$ the Schrödinger's equation can be written as

$$-\frac{\hbar^2}{2m} \left(\frac{\chi''_{n\ell'}}{\chi_{n\ell'}} + \frac{R''_p(r)}{R_p(r)} + 2 \frac{\chi'_{n\ell'} R'_p(r)}{\chi_{n\ell'} R_p(r)} \right) = V_H + V_P + E_{n\ell'} + \Delta E_{n\ell'} \tag{7}$$

We endorse the detail of the calculation procedure of the theory over to our previous work [5-7]. By following the procedure, we can write the eigenvalues for different n values. The eigenvalue in the case of $n = 0$ is

$$E_{n=0,\ell'} = -\frac{mB^2}{2\hbar^2(\ell'+1)^2} + \frac{2m^2B^3}{\hbar^3(2\ell'+1)(\ell'+1)^3} + \frac{2^{-\kappa} C \hbar^{2\kappa+1} (\ell'+1)^\kappa (2+2\ell'+\kappa)!}{(Bm)^\kappa (2+2\ell')!} \tag{8}$$

The eigenvalue in the case of $n = 1$ is

$$\begin{aligned} E_{n=1,\ell'} &= -\frac{mB^2}{2\hbar^2(\ell'+2)^2} + \frac{2m^2B^3}{\hbar^3(2\ell'+1)(\ell'+2)^3} \\ &+ \frac{2^{-\kappa-1} C \hbar^{2\kappa+1} (\ell'+2)^{\kappa-1} (2+2\ell'+\kappa)! (4+2\ell'+3\kappa+p^2)}{(Bm)^\kappa (2+2\ell')!} \end{aligned} \tag{9}$$

For $n = 2$, the eigenvalue is

$$\begin{aligned} E_{n=2,\ell'} &= -\frac{mB^2}{2\hbar^2(\ell'+3)^2} + \frac{2m^2B^3}{\hbar^3(2\ell'+1)(\ell'+3)^3} \\ &+ \frac{2^{-\kappa-2} C \hbar^{2\kappa+1} (\ell'+3)^{\kappa-1} (2+2\ell'+\kappa)!}{(Bm)^\kappa (3+2\ell')!} \\ &\times \left(36 + 8\ell'^2 + \kappa(3+\kappa)(14+\kappa(3+\kappa)) + 4\ell'(9+2\kappa(3+\kappa)) \right) \end{aligned} \tag{10}$$

These equations of eigenvalues for the first three n values are obtained by solving some integrals of which the detail has been explained in our previous study [5]. All analytical calculations have been performed by Mathematica. By paying close attention to the equations Eqs. 8-10 and the energies for higher n values, one can easily notice that the eigenvalues are changing on a regular basis. With the aid of this order, we can write a simple closed analytical form of the energy as following

$$\begin{aligned} E_{n,\ell} &= -\frac{mB^2}{2\hbar^2(n+\ell+1)^2} + \frac{2m^2B^3}{\hbar^3(2\ell+1)(n+\ell+1)^3} \\ &+ \frac{2^{-\kappa-n-1} C \hbar^{2\kappa+1} (n+\ell+2)^{\kappa-1} (2+2\ell+\kappa)!}{(Bm)^\kappa (n+2\ell+2)!} \end{aligned} \tag{11}$$

where the potential describes the Coulomb interaction for $C = 0$ while it depicts the harmonic oscillator behaviour for $\kappa = 2$ and $B = 0$.

2.2. The Asymptotic Iteration Method (AIM)

In this part, we give the information about AIM used in our calculations. AIM is an analytical technique which has been introduced to solve the second-order differential equations in the form of [20-23]

$$y'' = \lambda_0(x)y' + s_0(x)y \tag{12}$$

where $\lambda_0(x) \neq 0$, $s_0(x)$ and $\lambda_0(x)$, are differentiable variables. Eq. 12 has a general solution [20]

$$y(x) = e^{-\int^x \alpha(x')dx'} \left[C_2 + C_1 \int^x e^{\int^{x'} [\lambda_0(x'') + 2\alpha(x'')] dx''} dx' \right] \tag{13}$$

where in the case of sufficiently large $k > 0$, $\alpha(x)$ reads

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x), \quad k = 1, 2, 3, \dots \tag{14}$$

where

$$\begin{aligned} \lambda_k(x) &= \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x) \\ s_k(x) &= s'_{k-1}(x) + s_0(x)\lambda_{k-1}(x), \quad k = 1, 2, 3, \dots \end{aligned} \tag{15}$$

Recurrence relations also can be used by starting from $k = 0$ with the initial conditions $\lambda_{-1} = 0$ and $s_{-1} = 0$ [22]. A radial Schrödinger equation with a given potential is transformed into the form of Eq. 12. After determining $s_0(x)$ and $\lambda_0(x)$, one can find the parameters $s_k(x)$ and $\lambda_k(x)$, parameters by using the recurrence relations which are given in the Eq. 15.

The eigenvalues are calculated according to the Eq. 14. The Eq. 15 can also be written as

$$\delta_k(x) = \lambda_k(x)s_{k-1}(x) - \lambda_{k-1}(x)s_k(x) = 0 \quad k = 1, 2, 3, \dots \tag{16}$$

which equation can be used if the problem is exactly solvable. In the case of non-solvable case, we choose a suitable x_0 point for a specific n principal quantum number which is maximum value of the asymptotic wave function or the minimum value of the potential. The approximate energy eigenvalues are calculated from this equation for sufficiently great values of k with iteration.

In order to generate the eigenfunctions, one needs to use the following equation

$$y_n(x) = C_2 e^{-\int^x \frac{s_k(x')}{\lambda_k(x')} dx'} \tag{16}$$

where $k > n$, n and k correspond to the radial quantum and iteration numbers, respectively. For exactly solvable potentials, n is equal to k . Because nontrivial potentials do not have an exact solution, k is always greater than n in these numerical solutions and the approximate energy eigenvalues are obtained from the Eq. 16 in the case of sufficiently great values of k by iteration.

3. Results

In the present study, in order to make a comparative study, we have obtained the energy eigenvalues numerically for different A, B and C values in $\kappa = 1$ and $\kappa = 2$ cases. With some particular values of the parameters, in Figs. 1 and 2 it is possible to see the change of the ground state energy eigenvalues of the hydrogen atom in the $V(r) = C r^2$ potential, where $A = 0$, $B = 1$, $\kappa = 2$, $m = 1$ and $\hbar = 1$. We

have seen that the analytical results have close agreement with the AIM results for small quantum numbers.

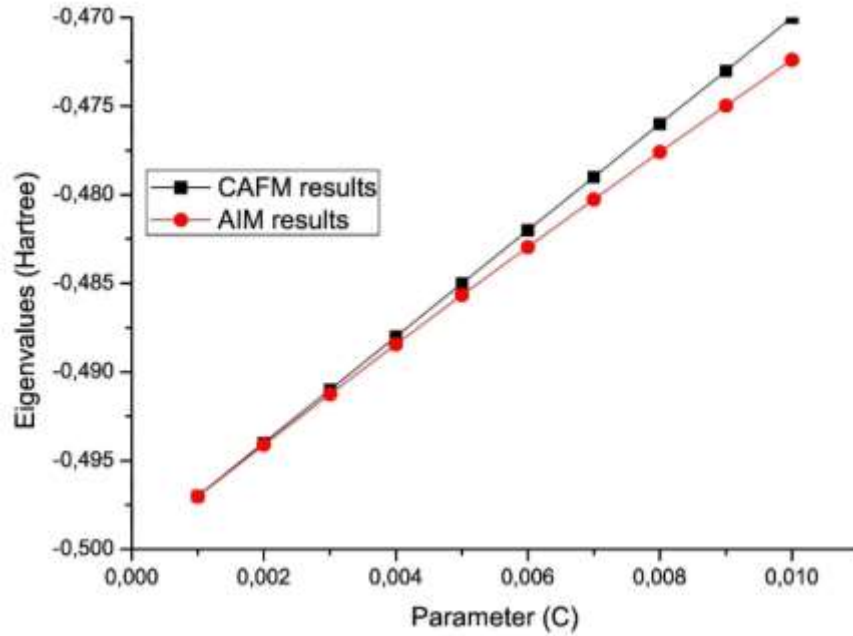


Figure 1. The comparison of the ground state energies obtained by CAFM and AIM methods.

As seen from the Fig. 1, two methods are giving similar results. However, in the case of increasing in parameter C , the results of two methods have different values. It can be considered such that the approximation in CAFM is stronger than that of AIM because CAFM is only aiming to get a perfect analytical expression to obtain the trend of the eigenvalue.

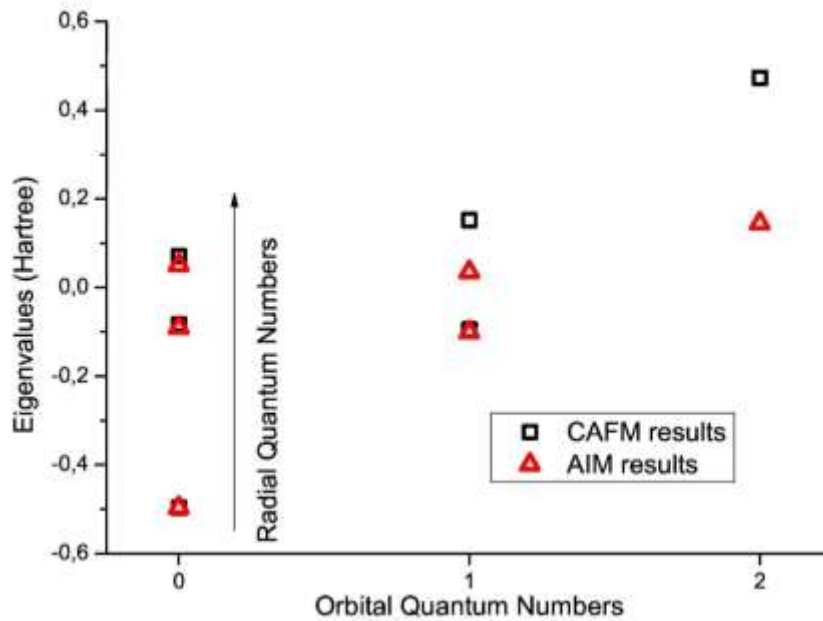


Figure 2. In the case of $C = 0.001$, the comparison of the results of CAFM and AIM methods for different quantum numbers.

Table 1. Comparison of our results with the numerical ones for energy eigenvalues of the potential family where $A=0.01, B=1, \kappa = -2, -1, 0, 1, 2, m=1$ and $\hbar = 1$.

κ	A	$\ell = 0$					
		$n = 0$		$n = 1$		$n = 2$	
		$E_{Anal.}$	E_{Num}	$E_{Anal.}$	E_{Num}	$E_{Anal.}$	E_{Num}
-2	0	-0.4980	-0.498068	-0.12475	-0.124758	-0.055481	-0.0554461
-1	0	-0.4990	-0.499044	-0.12475	-0.124755	-0.055444	-0.0554839
0	0	-0.4990	-0.499044	-0.12400	-0.124005	-0.054555	-0.0545572
1	0	-0.4985	-0.498546	-0.11900	-0.119068	-0.042055	-0.0426312
2	0	-0.4970	-0.497075	-0.08900	-0.090590		0.0507427
-2	0.01	-0.4780	-0.479293	-0.122250	-0.122370	-0.054707	-0.0547724
-1	0.01	-0.4790	-0.480131	-0.122250	-0.122357	-0.054703	-0.054732
0	0.01	-0.4790	-0.480093	-0.121500	-0.121602	-0.053814	-0.05384
1	0.01	-0.4785	-0.479546	-0.116500	-0.116561	-0.041314	-0.0417698
2	0.01	-0.4770	-0.477940	-0.080500	-0.087209		0.0529242

Table 2. Comparison of our results with the numerical ones for energy eigenvalues of the potential family where $A=0.01, B=1, \kappa = -2, -1, 0, 1, 2, m=1$ and $\hbar = 1$.

κ	A	$n = 0$		$n = 1$		$n = 2$	
		$\ell = 1$		$\ell = 1$		$\ell = 2$	
		$E_{Anal.}$	E_{Num}	$E_{Anal.}$	E_{Num}	$E_{Anal.}$	E_{Num}
-2	0	-0.124917	-0.124916	-0.055530	-0.055530	-0.019676	-0.019236
-1	0	-0.124750	-0.12475	-0.055444	-0.055444	-0.019960	-0.019195
0	0	-0.124000	-0.123999	-0.054555	-0.054555	-0.019000	-0.018240
1	0	-0.120000	-0.120057	-0.043055	-0.043617	-0.0145000	-0.008067
2	0	-0.095000	-0.100522		0.035599		
-2	0.01	-0.124083	-0.124090	-0.055284	-0.055285	-0.019964	-0.019196
-1	0.01	-0.123917	-0.123924	-0.055197	-0.055199	-0.019928	-0.019155
0	0.01	-0.123167	-0.123172	-0.054308	-0.054309	-0.014532	-0.018200
1	0.01	-0.119167	-0.119200	-0.042808	-0.043328	-0.041314	-0.0081283
2	0.01	-0.094166	-0.099469	0.036233		0.216440	

In the Tables 1 and 2, we show the obtained eigenvalues for the different κ values in the case of $A = 0$ or $A = 0.01$ and $C = 0.001$. We compare the values with the numerical results which is obtained by shooting method. For the small values of A and C , the values are very close to the numerical values.

In the Figs. 1 and 2, we show the obtained eigenvalues for the different κ values in the case of $A = 0$ or $B = 1$ and for different B values. We compare the values with that from AIM method which has been introduced previously. The results are almost consistent with each other. However, for the large values of quantum numbers, the consistency is vanishing.

In the Tables 1 and 2, we calculate the eigenvalues for the potential family in the case of $A = 0$ or $A = 0.01$ and $C = 0.001$. Here the parameter κ between -2 and 2 . We compare the eigenvalues with the results from numerical calculation which has been obtained by performing shooting method for the Schrödinger equation.

As can be seen from the tables and figures, the eigenvalues are close to the values obtained by numerical calculations. But as indicated before, the aim of the study is not to find exact solution, but to determine an analytical formulation for eigenvalues in order to see the trend of the variation with the quantum numbers and potential parameters.

4. Conclusion

AIM and CAFM have been used as approximation methods for the calculation of non-solvable potential family. Because of the numerical treatment, the AIM is able to predict the eigenvalues which are consistent with that obtained by numerical ones. Differently, main idea of the CAFM method is not finding an exact eigenvalue for the non-solvable potentials, but to obtain a closed analytical form of the eigenvalues and to give a well described relationship between potential parameters, quantum numbers and energy eigenvalues.

This potential family has been previously treated by using AIM and obtained successful results. But it is very hard to show a pure analytical expression by just using this method. By using CAFM, we would like to provide an analytical eigenvalue which cannot be obtained by AIM, at least for small C values.

Therefore, the equation Eq. 11 is describing the ground state energy values of a single particle trapped in potential family. We believe that this work will lead to another studies aiming to solve the non-solvable potentials and obtain closed analytical expressions of eigenvalues.

Author's Contributions

The author gave final approval of the current version and any revised version to be submitted to the journal.

Statement of Conflicts of Interest

No potential conflict of interest was reported by the authors.

Statement of Research and Publication Ethics

The authors declare that this study complies with Research and Publication Ethics.

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