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| RESEARCH ARTICLE

A Numerical Approach to Bound-State Eigenvalues of the One-Dimensional Finite Square Quantum Well

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| ABSTRACT

The one-dimensional finite quantum well is one of the fundamental problems in quantum mechanics, illustrating the formation of bound states, the penetration of the wave function into classically forbidden regions, and the quantization of energy. Unlike the infinite potential well, the finite quantum well requires the solution of transcendental equations, which cannot be solved analytically. This study presents the derivation of the transcendental equations for a finite quantum well, and their numerical solution through an implementation in the Fortran programming language. The transcendental equations were derived by analyzing the Schrödinger equation inside and outside the potential well. These equations were then solved using the Newton–Raphson method, leading to the development of an algorithm for determining the energies of the bound states. The algorithm was implemented as a Fortran program and compiled to obtain the roots of the transcendental equations for a quantum well of 4 ev depth and 2nm width, which were subsequently used to calculate the corresponding energy eigenvalues. The obtained results show excellent agreement with theoretical predictions. This efficient and portable implementation is suitable for educational and research applications in computational physics.

| KEYWORDS

Finite well, Numerical methods, Newton–Raphson, Transcendental equations.

| ARTICLE INFORMATION

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1. Introduction

The Schrödinger equation, as the fundamental equation of non-relativistic quantum mechanics, is a basic formula for describing the behavior of microscopic particles and investigating the quantum states of physical systems[1], [2]. Solving this equation for different potentials makes it possible to determine the energy levels and wave functions of particles[3]. One of the important and widely applicable models in this context is the one-dimensional finite square potential well. Unlike the infinite potential well, it allows the wave function to penetrate into the regions outside the classically allowed region and demonstrates the phenomenon of quantum tunneling. By solving the Schrödinger equation for this system and applying the continuity conditions of the wave function, relations for the even and odd states are obtained. Due to their nonlinear nature and the presence of trigonometric functions, these relations are known as transcendental equations[4], [5]. These equations do not have analytical solutions, and determining the allowed energy levels of the bound states requires the use of numerical methods to find their roots[6].The finite potential well is one of the earliest quantum models studied for investigating the properties of quantum systems following the formulation of the Schrödinger equation by Erwin Schrödinger in 1926 [5]. Early studies in this field focused mainly on deriving theoretical relationships, determining the conditions for the existence of bound states, and analyzing the qualitative behavior of energy levels[7]. With the development of computational methods, various numerical techniques, such as the Bisection, Newton–Raphson, and Secant methods, have been employed to solve nonlinear equations and determine the energy eigenvalues. Previous studies have shown that these methods have broad applications in the analysis of both simple and complex quantum systems, particularly in structures such as quantum wells,

semiconductors, quantum dots, and nanoscale systems[8], [9], [10]. Furthermore, with advances in computational science, scientific programming languages such as Fortran, MATLAB, and Python have become effective tools for implementing numerical algorithms and analyzing problems in quantum mechanics.

However, many studies have focused on solving quantum systems using numerical methods and computer programming[11]. Nevertheless, no specific study has yet been reported that theoretically investigates the finite potential well and, through the analysis of the corresponding equations using numerical methods, provides their roots in an accessible form. Therefore, obtaining accurate values of the energy levels in this well has remained a major challenge.

In this study, the one-dimensional finite square potential well is investigated by numerically solving the transcendental equations corresponding to the even and odd states. For this purpose, a computational program is developed in the Fortran environment that is capable of calculating the roots of the transcendental equations using the Newton–Raphson method by taking parameters such as the potential well depth, well width, particle mass, and the number of desired states as inputs. The allowed energies of the bound states are then determined. The computational results are stored in appropriate files to facilitate the analysis and plotting of the energy levels. In addition to providing an accurate numerical approach for solving one of the fundamental problems in quantum mechanics, this approach practically demonstrates the connection between the theoretical concepts of quantum physics and computational methods and can serve as an educational and research framework for investigating similar quantum systems.

2. Methods

This study is theoretical and computational in nature and is conducted with the aim of determining the energy levels of particles in a one-dimensional finite potential well. First, the time-independent Schrödinger equation for the finite potential well is derived and solved in the different potential regions. Then, by applying the continuity conditions of the wave function and its derivative at the boundaries of the well, the transcendental equations governing the even and odd states are obtained. In the next step, the Newton–Raphson numerical method is selected to determine the roots of the transcendental equations and calculate the energy eigenvalues. This method is employed because of its high convergence rate and suitable accuracy in solving nonlinear equations[12]. For the computational implementation, the equations are first transformed into a suitable form for the Newton–Raphson algorithm, and the required derivatives are then derived. Following the mathematical formulation of the problem, a computational program is developed using the Fortran programming language. In this program, the Newton–Raphson algorithm is implemented to determine the roots of the transcendental equations, and the energy eigenvalues are calculated for different potential-well parameters. Finally, the obtained numerical results are analyzed, and the allowed energy levels of the system are extracted and examined. This study consists of three main stages: (1) theoretical analysis and derivation of the governing equations for the finite potential well, (2) numerical solution of the transcendental equations using the Newton–Raphson method, and (3) implementation and analysis of the results using a program developed in Fortran 95.

3. Results and Discussion

3.1 Derivation of transcendental equations

A finite potential well with a potential depth of V_0 and a width of L=2a was considered. Its mathematical relation has shown as follows;

$$V(x)=\begin{cases}-V_0, & |x|<a,\\ 0, & |x|>a,\end{cases}$$

Graphical scheme of this well has demonstrated in figure 1.

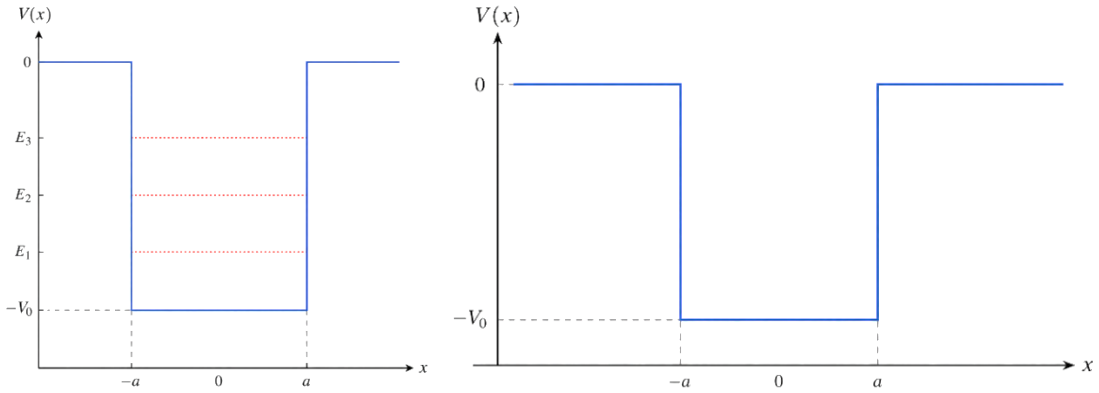


Figure 1: (a) Schematic representation of the potential well; (b) energy levels of the particle in the given well.

The one-dimensional Schrödinger equation is given as follows:

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}\big(E-V(x)\big)\psi(x)=0 \tag{1}$$

By considering this equation inside and outside the potential region $V(x)=0$ and $V(x)=-V_0$, it is obtained that:

$$\frac{d^2\psi(x)}{dx^2}-k^2\psi(x)=0 \qquad ;k=\sqrt{\frac{-2mE}{\hbar^2}} \tag{2}$$

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}(E+V_0)\psi(x)=0 \qquad ;l=\sqrt{\frac{2m(E+V_0)}{\hbar^2}} \tag{3}$$

The solution of equation 2 is

$$\psi(x)=A\,e^{kx}+B\,e^{-kx}$$

At $x<-a$ region with $x\to-\infty$ we have

$$\psi(x)=A\,e^{kx} \tag{4}$$

However, if we consider $x>a$ region and the solution is written as

$$\psi(x)=C\,e^{kx}+D\,e^{-kx}$$

By applying $x\to\infty$ we get

$$\psi(x)=D\,e^{-kx} \tag{5}$$

On the other hand, the solution of equation 2 is

$$\psi(x)=E\sin(lx)+F\cos(lx) \tag{6}$$

Considering the continuity condition at boundaries; for example, at $x=a$ we have

$$D\,e^{-kx}=E\cos lx \tag{7}$$

By taking the derivates from both sides

$$-k\,D\,e^{-kx}=-l\,E\sin lx$$

And, deviding the results on equation 7 we obtain

$$k=l\tan la$$

If $z=la$ is substituted then

$$ka=z\tan z \tag{8}$$

And upon calculating the value, we obtain

$$k^2 + l^2 = \frac{2mV_0}{\hbar^2} \;;\; (ka)^2 = a^2\frac{2mV_0}{\hbar^2} - (la)^2$$

$$ka = \sqrt{R^2 - z^2} \quad ; \quad R = a\sqrt{\frac{2mV_0}{\hbar^2}} \tag{9}$$

By putting equation 9 in equation 8, the bound state equations is obtained:

$$\tan z = \sqrt{\frac{R^2}{z^2} - 1} \qquad \text{(even states)} \tag{10}$$

And similarlyl, considering $x = -a$, it is obtained for odd states

$$-\cot z = \sqrt{\frac{R^2}{z^2} - 1} \qquad \text{(odd states)} \tag{11}$$

By solving the transcendental equation and finding of Z_n , the energy value is

$$E_n = \frac{\hbar^2 z_n^2}{2ma^2} - V_0 \tag{12}$$

As it is clear from equation 12, the energies are depending on Z_n[5].

3.2 Numerical solution

The equations of 10 and 11, were obtained for the one-dimensional finite potential well in the even and odd states, respectively.

The Newton–Raphson method was employed. For the even states

$$f(z) = \tan z - \sqrt{\frac{R^2}{z^2} - 1} = 0$$

Its derivative is given as

$$\acute{f}(z) = \sec^2 z + \frac{R^2}{z^3\sqrt{\frac{R^2}{z^2} - 1}}$$

Based on the theory and the Newton–Raphson equation, the root-finding iteration is given as follows:

$$z_{n+1} = z_n - \frac{\tan z_n - \sqrt{\frac{R^2}{z_n^2} - 1}}{\sec^2 z_n + \frac{R^2}{z_n^3\sqrt{\frac{R^2}{z_n^2} - 1}}}$$

At the same time, for the odd states, it was obtained that:

$$f(z) = -\cot z - \sqrt{\frac{R^2}{z^2} - 1} = 0$$

Its derivative is given as

$$\acute{f}(z) = csc^2 z + \frac{R^2}{z^3\sqrt{\frac{R^2}{z^2} - 1}}$$

Based on the theory and the Newton–Raphson equation, the root-finding iteration is given as follows:

$$z_{n+1} = z_n - \frac{-\cot z_n - \sqrt{\frac{R^2}{z_n^2} - 1}}{csc^2 z_n + \frac{R^2}{z_n^3\sqrt{\frac{R^2}{z_n^2}-1}}}$$

As the process of finding roots repeats the z_{n+1} becomes close to the absolute root[12]. After obtaining the root Z_n, the following equation was added to the Fortran code to calculate the energy formula:

$$E_n = -V_0 + \frac{\hbar^2 z_n^2}{2ma^2}$$

This equation was used to calculate the energies of the bound states[5], [6]. For each root Z_n, a corresponding energy E_n was calculated.

3.3 Fortran Implementation

Based on the transcendental equations for the finite potential well and the Newton–Raphson method formulated previously, a flowchart was developed for writing an efficient and effective program to determine the roots of the equations and subsequently calculate the energy levels (Figure 2).

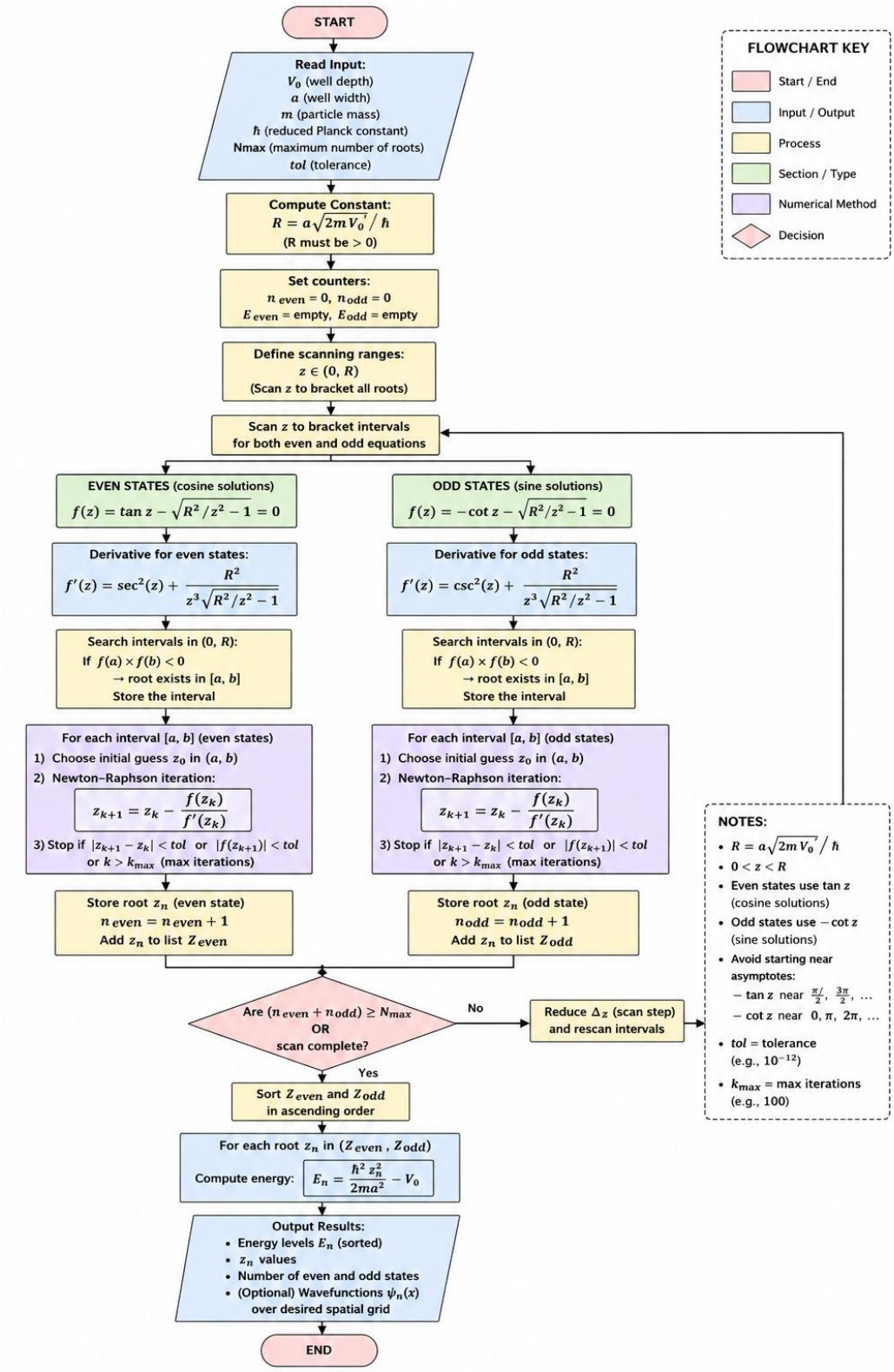


Figure 2: Flowchart for solving the transcendental equations in Fortran 95 and determining the energy eigenvalues.

This flowchart consists of input, analysis, decision-making, computation, and output sections. Based on this flowchart and the specific algorithms developed, the required code was written in the Fortran environment (Table 1).

Table 1: A fortran 90 code for solving of transcendental equations of 1D-finite potential well.

Input part (V_0, a, m, $\hbar$ and a tolerance value for root recognition).	program finite_potential_well implicit none real::a,m,v,h,tol,r,fz,z,gz,znew,E,k(10),p(10),x(10),n(10) integer::i,j,l a=1E-9 V=6.4E-19 tol=0.001 m=9.1E-31
Computing of constants: R	h=1.05E-34 r=a*sqrt(2*m*v/h**2) write(*,*)"R=",r
Initial values for even roots	
	x(1)=1.4 x(2)=4.2 x(3)=6.8 x(4)=9.5 write(*,*)"The even roots and corresponding energy eigenvalues are:" do l=1,4 z=x(l)
	do i=1,1000
	fz=tan(z)-sqrt(((r**2)/(z**2))-1)
	gz=((1/cos(z))**2)+((r**2)/((z**3)*sqrt(((r**2)/(z**2))-1)))
	znew=z-(fz/gz)
Even states (Cosine solutions)	if (abs(znew-z)<tol) then
	p(i)=znew
	E=(((h**2)*(znew**2)/(2*m*(a**2)))-v)*6.25E18
	k(i)=E
	write(*,*)"z=",p(i)
	write(*,*)"E=",k(i),"eV"
	exit
	else
	z=znew
	end if
	end do
	end do
Initial values for odd roots	
	n(5)=2.5 n(6)=5.3 n(7)=8.2
	write(*,*)"The odd roots and corresponding energy eigenvalues are:" do j=5,7 z=n(j)
	do i=1,1000
Odd states (sin solutions)	fz=-(1/tan(z))-sqrt(((r**2)/(z**2))-1)
	gz=((1/sin(z))**2)+((r**2)/((z**3)*sqrt(((r**2)/(z**2))-1)))
	znew=z-(fz/gz)
	if (abs(znew-z)<tol) then
	p(i)=znew
	E=(((h**2)*(znew**2)/(2*m*(a**2)))-v)*6.25E18
	k(i)=E
	write(*,*)"z=",p(i)
	write(*,*)"E=",k(i),"eV"
	exit
	else
Program end	z=znew
	end if
	end do
	end do end program finite_potential_well

Compilation of the written program yielded the roots of the transcendental equations for both even and odd states and subsequently provided the corresponding values of the energy levels, which are listed in the table below. Note that, it was tried to make the code as simple as possible for understanding.

Table 2: Obtained roots of the transcendental equations and their corresponding energy levels.

No.	State Type	Root	Energy E (eV)
1	Even	1.43	−3.922
2	Odd	2.85	−3.69
3	Even	4.28	−3.305
4	Odd	5.69	−2.77
5	Even	7.09	−2.095
6	Odd	8.45	−1.29
7	Even	9.74	−0.402

In addition, the obtained transcendental equations, taking into account the value of R, which was determined to be approximately 10.278 from the compilation of the code written in the Fortran environment, were plotted using Gnuplot to visually verify that the obtained roots lie within the corresponding regions (Figure 3).

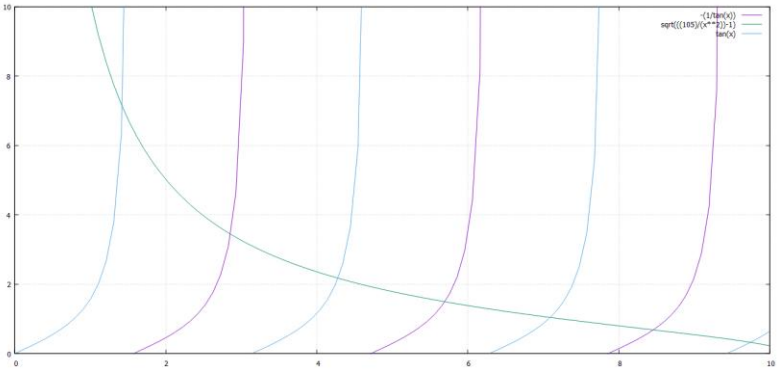
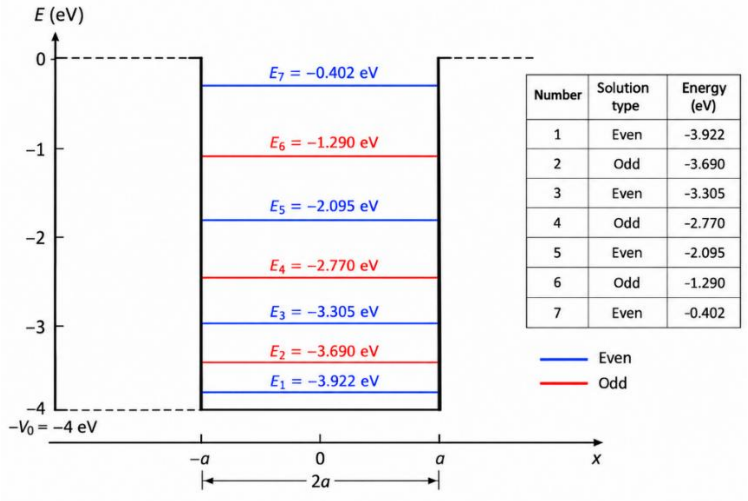


Figure 3: Plotting of the transcendental equations using the Gnuplot software.

In the above figure, the functions tan(x), -cot(x) and $\sqrt{\frac{R^2}{z^2}-1}$ are plotted together, where the obtained roots can be clearly observed. Furthermore, the energy levels in the given potential well are plotted, with the first energy level located close to the bottom of the well and the highest energy level close to the top of the well (Figure 4). This observation further confirms the correctness of the analysis of the problem and enhances the reliability of the calculations.



Number	Solution type	Energy (eV)
1	Even	-3.922
2	Odd	-3.690
3	Even	-3.305
4	Odd	-2.770
5	Even	-2.095
6	Odd	-1.290
7	Even	-0.402

Figure 4: Energy-level diagram of the finite potential well with a depth of −4 eV and a width of 2 nm.

As shown in Figure 4, the electron can have seven bound energy states in this well, including four even states and three odd states.

4. Discussion

The results obtained from this study demonstrate that numerical methods play a crucial role in solving problems in quantum mechanics. The transcendental equations derived from the boundary conditions of the finite potential well do not have direct analytical solutions[7]; therefore, the Newton–Raphson method was applied to accurately determine the roots of these equations and, consequently, the allowed energy levels. The computational results showed that increasing either the depth or the width of the potential well leads to an increase in the number of bound states and allowed energy levels, which is fully consistent with the theoretical predictions of quantum mechanics[13].

One of the important findings of this study is the high efficiency of the Newton–Raphson method compared with many other iterative methods[14]. When an appropriate initial value is selected, this method converges rapidly toward the solution and provides satisfactory accuracy in determining the energy eigenvalues. However, the results showed that an inappropriate choice of the initial value may lead to convergence toward an undesired root or even cause the algorithm to fail to converge. Therefore, careful selection of the initial values is an important factor in the successful application of this method[15].

Despite the successful performance of the method employed, this study has several limitations. First, the study was limited to a one-dimensional finite potential well, and the effects of two- and three-dimensional systems were not investigated. Second, only the Newton–Raphson method was used for the main calculations, and no comprehensive comparison was conducted between its performance and that of other numerical methods, such as the Bisection, Secant etc. Furthermore, the studied system was assumed to be ideal, and factors such as particle interactions, external fields, and environmental perturbations were not considered.

The implications of this study extend beyond the solution of an educational problem in quantum mechanics. The proposed method can be applied to the analysis of semiconductor structures, quantum wells, nanostructures, and other quantum systems. In addition, the implementation of the algorithm in Fortran 95 can serve as a model for developing more advanced computational programs in computational physics and engineering. The results of this study also demonstrate that combining numerical methods with scientific programming provides an effective tool for solving complex problems for which analytical solutions are difficult or impossible to obtain.

Overall, the findings of this study, while confirming the theoretical foundations of quantum mechanics, demonstrate that the Newton–Raphson method is a suitable and reliable tool for solving the transcendental equations of a finite potential well and extracting the corresponding energy levels. However, extending the study to more complex systems and comparing different numerical methods could provide a basis for obtaining more accurate results and broader applications in future studies.

4. Conclusion

In this study, the one-dimensional finite potential well was investigated as one of the fundamental problems in quantum mechanics. First, using the time-independent Schrödinger equation, the wave functions in the different regions of the well were derived, and by applying the appropriate boundary conditions, the transcendental equations corresponding to the even and odd states were obtained. Since these equations do not have direct analytical solutions, the use of numerical methods is necessary to determine the energy eigenvalues.

The results of the study showed that the equations of the finite potential well can be solved by transforming them into a root-finding problem and subsequently applying numerical methods. Among the various methods, the Newton–Raphson method is considered one of the most efficient approaches for finding the roots of transcendental equations because of its high convergence rate and suitable accuracy. In addition, methods such as the Bisection, Secant, and Fixed-Point Iteration methods can also be used to solve these equations.

It was also found that, by obtaining the roots of the transcendental equations, the dimensionless parameters of the problem can be determined, and the energy eigenvalues can be readily calculated through the physical relationships between these parameters and the energy. In other words, each valid root of the transcendental equation corresponds to an allowed quantum state and determines its associated energy eigenvalue. Therefore, finding the roots represents a key step in determining the energy levels of a finite potential well.

The implementation of the Newton–Raphson algorithm in the Fortran 90 environment demonstrated that this programming language has a high capability for performing numerical calculations and can determine the allowed energy

levels with satisfactory accuracy and low computational time. Overall, the results of this study indicate that combining theoretical analysis of the Schrödinger equation with numerical methods provides an effective and reliable approach for studying quantum systems and calculating energy levels in finite potential wells.

Autor contributions

The concept of the study was established by Sayed A. S. Mosamem, who also developed the Fortran code for solving of transcendental equations. Moreover, he created the first draft of manuscript. Mohammad Muhsen Hewadmal was contributed by analyzing of theoretical concepts, writing of literature review and developing of the corresponding newton-Raphson algorithm. Khudaidad Wasiq was contributed by setting of the methods, preparing of tables, charts and finalizing of the manuscript.

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