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Modeling Time-Independent Schrödinger Equation for an Infinite Potential Well Using Numerov and Matrix Methods

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Highlights

- **Time Independent Schrödinger Equation (TISE) has been solved numerically for an infinite potential square well in one dimension.**
- **Two approximation methods, Numerov and Matrix methods have been employed to find the energy eigenvalues and wave functions for the particle inside the infinite square well potential.**
- **By comparisons with exact analytical solutions, the validity and accuracy of the two methods have been demonstrated.**
- **The merits of these numerical methods are to avoid a huge expense in time when solving Schrödinger Equation.**

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ABSTRACT

The objective of this study is to numerically solve and apply two approximate methods to investigate the Time Independent Schrödinger Equation (TISE) in one dimension for an infinite potential square well. These two numerical methods are the Numerov Method (NM) and Matrix Method (MM). As a simulation tool, MATLAB, a high-level programming language and an efficient simulation tool, is used for modeling and solving TISE in one dimension. Exact analytical solutions for these potential functions are obtained and compared with numerical solutions and computational techniques. The energy eigenvalues and Eigen functions of a particle (such as an electron) restricted to move inside this potential are discussed as an illustration. The numerically calculated energies of several states with increasing numbers of points were obtained from both methods and compared with the simulation results of the exact solution. As an exemplary case, the first five wave functions are accurately determined numerically where the discreteness is found since the wave function vanishes at the boundary. The obtained results show very good agreement and the similarity is clearly confirmed between the three cases. This agreement confirms that this approach was highly accurate and efficient. The accuracy and the convergence of the numerical obtained results were easily checked. The stability of these methods is due to the fact that there are no restrictions on the time steps to be taken. The merits of these numerical methods are to avoid a huge expense in time when solving Schrödinger equation.

1. Introduction

There are numerous fundamental equations for representing quantum mechanical behavior in material science. The progress of quantum mechanics at the beginning of the twentieth century occurred as a shock to the physics community at that time. In spite of the great successes of quantum mechanics and a century that has passed since its introduction, quantum mechanics was initially questioned due to its limitation regarding non-relativistic particles and arguments still continue about its meaning and its future (Weinberg, 2017). Niels Bohr said, "If you are not confused by quantum physics then you haven't understood it". Richard Feynman also remarked, "I think I can safely say that nobody understands quantum mechanics" (Griffiths, 2005). As Griffiths says in his book that quantum mechanics does not flow smoothly and naturally from earlier theories, but, on the contrary, it represents an abrupt and revolutionary departure from classical ideas (Griffiths, 2005). The most significant equation among these is the Schrödinger equation which is employed to explain the variations of quantum system with time (Arora *et al*., 2019). Erwin Schrödinger developed this linear partial differential equation of second order to explain the wave nature of matter and particles associated with the wave. This equation is called as Schrödinger Equation (SE) (Griffiths, 2005; Arora *et al*., 2019; Schrödinger, 1926; Serway *et al*., 2005). It is analogous to the wave equation in optics which is centered on the assumption that a particle behaves as a wave. The solution of the Schrödinger Equation contains both the wave function (ψ) and the energy (E) of the particle under consideration. The wave function ψ is most important because when the wave function is obtained, everything about the particle can be known. For example, the probability of finding the particle in a particular region at a position x (within a region of length dx) at a particular instant of time t can be expressed by the absolute square of Ψ , $|\psi(x,t)|^2$. The energy of the particle (E) depends on the potential V and the boundary conditions. These are very important parameters (constraints on the particle) and they are either quantized or continuous. Depending on its dependency on time, Schrödinger equation can be classified under two headings: Time-dependent Schrödinger equation (TDSE) and Time independent Schrödinger equation (TISE) (Barde *et al*., 2015). The Schrödinger equation can be thought of as playing a role equivalent to Newton's second law, where $\psi(x,t)$ is determined for all future times by the Schrödinger equation; exactly as Newton's law determines *x(t)* for all future time (Griffiths,

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2005). Even though, the Schrödinger equation has been constantly solved numerically using different methods (Bhatia and Mittal, 2018; Yadav and Jiwari, 2019; Ledoux and Van Daele, 2014; Ma and Chen, 2009; He and Lin, 2020; Ward and Volkmer, 2006; Pitkanen, 1955), the need for simple and less complicated methods are desired. For this aim, the following sub-sections discuss briefly both main types of Schrödinger equation in some detail.

1.1. Time-Dependent Schrödinger Equation

When a particle has a fixed energy E, its wave function could be written in the following form:

$$\psi(x,t) = Ae^{i(kx-\omega t)} \tag{1}$$

where A is the amplitude of the wave and ω is the angular frequency.

Eq. (1) represents a wave travelling in the positive x direction, and it is a wave function for a free particle of momentum $p = \hbar k$ and energy $E = \hbar\omega$. The second derivative for $\psi(x,t)$ with respect to x is:

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = -k^2\psi(x,t) \tag{2}$$

Energy can be written as:

$$E = p^2/2m = \hbar^2k^2/2m \tag{3}$$

where m is the mass of the particle, $\hbar$=h/2π, where h is Planck constant, p is the momentum, and k is the wave number.

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{p^2}{2m}\psi(x,t) \tag{4}$$

Similarly

$$\frac{\partial\psi(x,t)}{\partial t} = -i\omega\psi(x,t) \tag{5}$$

From $E = \hbar\omega$, and by substituting $\omega = E/\hbar$ in Eq. (5), the equation can be further modified to obtain:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = E\psi(x,t) \tag{6}$$

But the total energy is equal to sum of the kinetic energy and the potential energy V(x), hence:

$$E = \frac{P^2}{2m} + V(x) \tag{7}$$

and

$$E\psi(x,t) = \frac{\hbar^2}{2m}\psi(x,t) + V(x,t)\psi(x,t) \tag{8}$$

Consequently, the time dependent Schrödinger equation can be written in the form (Briggs and Rost, 2001; Hamdan *et al.*, 2022):

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{9}$$

1.2. Time Independent Schrödinger Equation

According to the classical description, total energy E can be written as in Eq. (7) and when multiplying both sides by ψ (x, t), Eq. (7) becomes:

$$E\psi(x,t) = \frac{p^2}{2m}\psi(x,t) + V(x,t)\psi(x,t) \tag{10}$$

The operator of momentum can be expressed as $P = -i\hbar d/dx$, and the wave function as $\psi = e^{i(kx-\omega t)}$, where k is the wave number (k=2π/λ).

Replacing p^2 and $d^2\psi(x,t)/dx^2 = -k^2\psi$ into Eq. (9), the following equation is obtained:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{11}$$

Eq. (11) represents the time independent Schrödinger equation in one dimension (Zettili, 2003). Typical examples in quantum mechanics that exemplify differences between classical and quantum mechanical situations are the square well and infinite well potentials (Barde *et al.*, 2015; Harrison, 2009). To this end and in this paper, this equation is solved and modeled for the infinite potential well using two approximation methods; Numerov Method (NM) and Matrix Method (MM).

2. Materials and Method

2.1. Infinite Potential Well

In this paper, the infinite potential well is chosen to solve the Time Independent Schrödinger Equation (TISE) in one dimension (see Fig. 1)

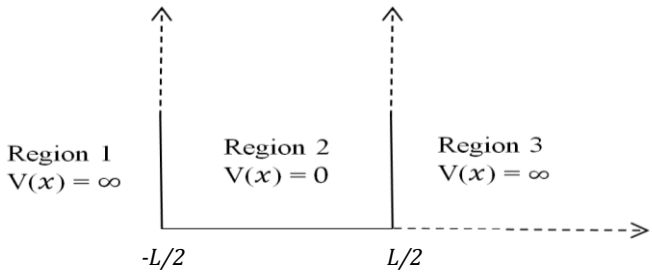


Fig. 1. The infinite square well potential.

Consider the potential energy:

$$V(x) = \begin{cases} 0, & -L/2 \le x \le L/2 \\ \infty, & x < -L/2 \text{ or } x > \frac{L}{2} \text{ (or otherwise)}, \end{cases} \tag{12}$$

The potential energy function V(x) is equal to zero within the well and Schrödinger Equation becomes:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{13}$$

Since the wave function $\psi(x)$, is continuous and is equal to zero within the walls of the well, the wave function approach zero as x approaches $-L/2$ or $+L/2$. The solution of Eq. (13) is required to satisfy the following boundary (constraints on the particle) conditions:

$$\psi(-L/2) = 0 \text{ and } \psi(+L/2) = 0 \tag{14}$$

Eq. (13) is rewritten and multiplied by $-2m/\hbar$ to obtain the following equation:

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2}\right)\psi = 0$$

Substituting

$$k^2 = \frac{2mE}{\hbar^2} \tag{15}$$

then the Schrödinger equation becomes:

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \tag{16}$$

Hence, the even and odd solutions of this equation have the following forms, respectively (i.e. the classical simple harmonic oscillator):

$$\psi(x) = A\cos(kx), for\ -L/2 \le x \le L/2 \tag{17}$$

$$\psi(x) = A\sin(kx), for\ -L/2 \le x \le L/2 \tag{18}$$

where A is a normalization constant.

The conditions imposed upon the even and odd solutions lead to the distinct solutions:

$$k = n\pi/L\ , with\ n = 1, 2, 3, \ldots \tag{19}$$

where n is an odd integer or an even integer, depending on the particular case with respect to the center of the well.

Hence, the possible values of the energy are obtained from Eq. (3). Written in terms of the integer n as:

$$E = n^2\pi^2\hbar^2/2mL^2 \tag{20}$$

This means that, in contrast to the classical problem, a particle in the infinite square well can have only one of these special allowed values and that energy quantization arises as a technical outcome of the boundary conditions on the solutions to the TISE. The lowest energy is the ground state and the other energies increasing in proportion to n^2 are the excited states. The probability of getting a specific energy is independent of time. This is just a manifestation of energy conservation in quantum mechanics. There is also no acceptable solution to the TISE for this well with E=≤0 (Griffiths, 2005).

For the normalization constant, the wave functions and the values of the energy of a particle moving in an infinite well depend upon a positive quantum number integer n. As the probability of finding the particle in an infinite well in the region between $-L/2$ and $+L/2$ must be equal to unity, therefore:

$$\int_{-L/2}^{+L/2} |\psi(x)|^2 dx = 1 \tag{21}$$

The even solutions for the particle in the infinite well can be obtained using Eq. (17) into Eq. (18), one gets an infinite set of solutions; one for each positive integer n:

$$\psi(x) = A\cos\left(\frac{n\pi x}{L}\right)$$

Substituting this equation into Eq. (21) gives:

$$A^2\int_{-L/2}^{+L/2} \cos^2\left(\frac{n\pi x}{L}\right) dx = 1$$

Using the identity,

$$\cos^2(x) = \frac{1}{2}[\sin^2(x) + \cos^2(x)] = \frac{1}{2}$$

the above equation becomes:

$$A^2\int_{-L/2}^{+L/2} 1/2\, dx = 1$$

Since the above integral has the value $L/2$, the following value for A is obtained:

$$A = \sqrt{L/2}$$

The normalization constant A for the odd functions can be shown to be given by the same equation. Using this result the wave function of a particle in an infinite well, with respect to the center of the well, can be written as:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right), & n\ odd\ (1,3,5,\dots) \\ \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), & n\ even\ (2,4,6,\dots) \end{cases} \tag{22}$$

In this part arbitrary potential width L=2 nm has been assumed. Taking the mass of the electron, m_e=5.6875×10^{-12} eV/C^2, and Planck constant, $\hbar$ =0.658 x 10^{-15} $eV.S$, the exact values of E in terms of n, for an electron in an infinite quantum well with a width 2 nm, is found to be:

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$E = \frac{n^2\pi^2 \times (0.658 \times 10^{-15})^2}{2 \times 5.6875 \times 10^{-12}(2 \times 10^{-9})^2}$$

2.2. Numerical Simulations

A code was written to solve the TISE using MATLAB, one of the efficient simulation tools commonly used to attain accurate solutions readily with the aid of short and easily constructed programming codes (Cooper, 2012). Tables 1 and 2 present the numerically calculated energies of the first six infinite square well states with an increasing number of points obtained from the Matrix and the Numerov Methods, where the simulation results are compared to the exact solution (Eq. (22)). As an exemplary case, the first five wave functions are accurately determined numerically. In the case of this infinite well, the discreteness is clear because $\psi = 0$ at the boundary, as shown in Fig. 2. The first five wave functions are shown in Fig. 2 as obtained from the Numerov and matrix methods and compared to the exact solution. The similarity is clearly confirmed between the three cases.

As can be seen from the above Tables, the numerical results obtained from the Matrix, and Numerov Methods are very close to the exact analytical solutions, particularly when the number of points is increased. Hence, as expected, this input parameter affects the results and increasing the number of points leads to the exact solution. For the eigenvalues, Table 3 shows a comparison of exact solution of energy eigenvalues for the first ten states, for an infinite well with width L=2 nm and number of points N=500, with the eigenvalues obtained from the NM and the MM. Fig. 3 shows graphically the comparison between the three methods.

Table 1

Numerically calculated energies of the first six infinite square well states with an increasing number of points obtained from Matrix Method and compared to the exact solution.

Solution	E_1 (eV)	E_2 (eV)	E_3 (eV)	E_4 (eV)	E_5 (eV)	E_6 (eV)
Exact Solution	0.0939	0.3757	0.8452	1.5027	2.3479	3.3809
Matrix Method solution (N=50)	0.0940	0.3746	0.8436	1.4962	2.3306	3.3434
Matrix Method solution (N=100)	0.0940	0.3760	0.8456	1.5024	2.3457	3.3748
Matrix Method solution (N=500)	0.0940	0.3769	0.8479	1.5044	2.3505	3.3846

Table 2

Numerically calculated energies of the first six infinite square well states with an increasing number of points obtained from Numerov's Method and compared to the exact solution.

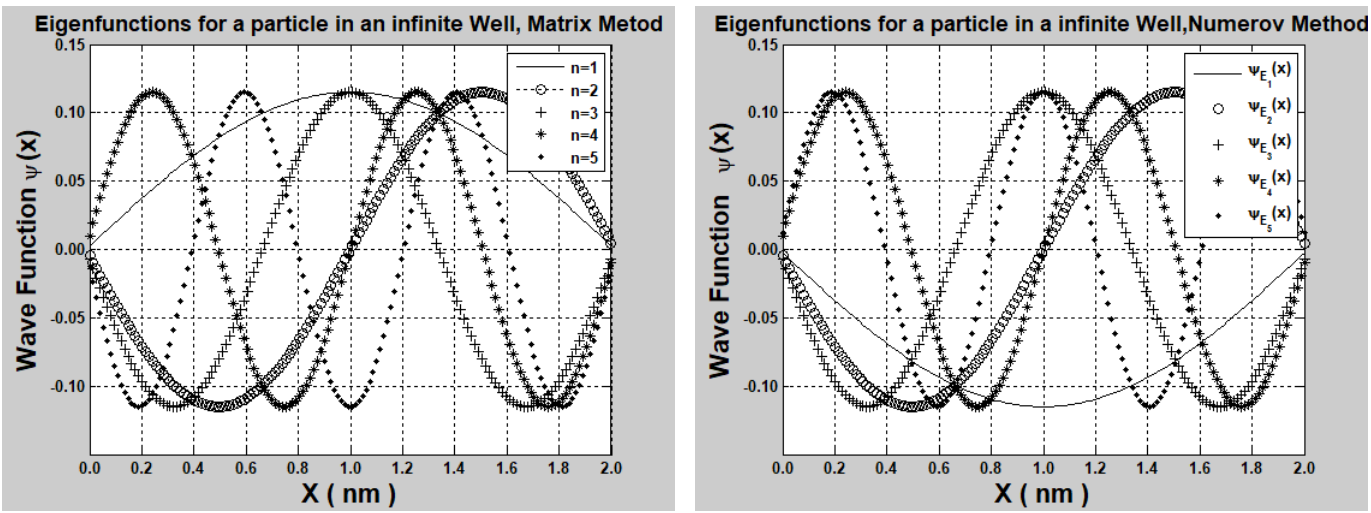
Solution	E_1 (eV)	E_2 (eV)	E_3 (eV)	E_4 (eV)	E_5 (eV)	E_6 (eV)
Exact	0.0939	0.3756	0.8452	1.5026	2.3479	3.3809
Numerov Method (N=50)	0.0868	0.3470	0.7795	1.3826	2.1542	3.0913
Numerov Method (N=100)	0.0904	0.3615	0.8130	1.4445	2.2554	3.2449
Numerov Method (N=500	0.0933	0.3733	0.8400	1.4933	2.3333	3.3598

Table 3

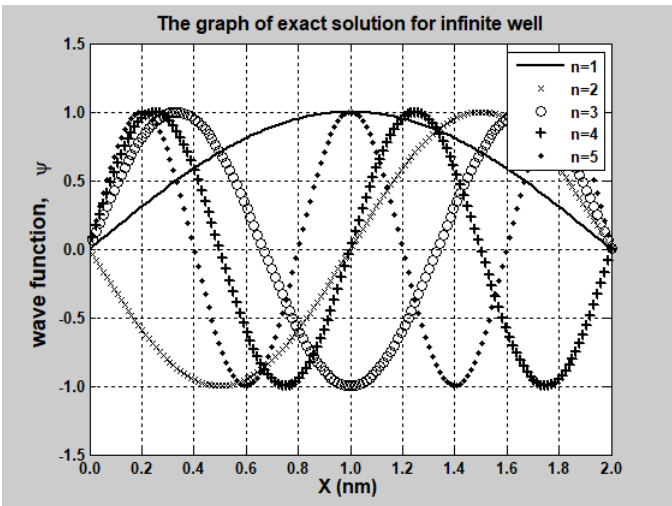
Comparison of the exact solution of energy eigenvalues for the first ten states for infinite well with width L=2 *nm*.

N point	Quantum Number n	Exact solution (eV)	Energy Eigenvalue (eV) (MM)	Energy Eigenvalue (eV) (NM)
500	1	0.0939	0.0942	0.0933
	2	0.3757	0.3769	0.3733
	3	0.8452	0.8479	0.8400
	4	1.5027	1.5044	1.4933
	5	2.3479	2.3505	2.3333
	6	3.3809	3.3846	3.3598
	7	4.6019	4.6158	4.5728
	8	6.0106	6.0285	5.9724
	9	7.6072	7.6294	7.5584
	10	9.3916	9.4185	9.3308

As can be seen from Table 3, the obtained results from the Matrix Method are in better agreement and very close to the exact solution results than those obtained from the Numerov Method. Hence, the validity and accuracy of the two methods are exhibited by the good agreement obtained. These results from the numerical simulations prove the advantages of the method. The stability of these methods is due to the fact that there are no restrictions on the time steps to be taken. The merits of these numerical methods are to avoid a huge expense in time when solving Schrödinger equation.



(a) (b)



(c)

Fig. 2. First five wave function for a particle in an infinite well using (a) Matrix Method (b) Numerov's Method and (c) Exact solution.

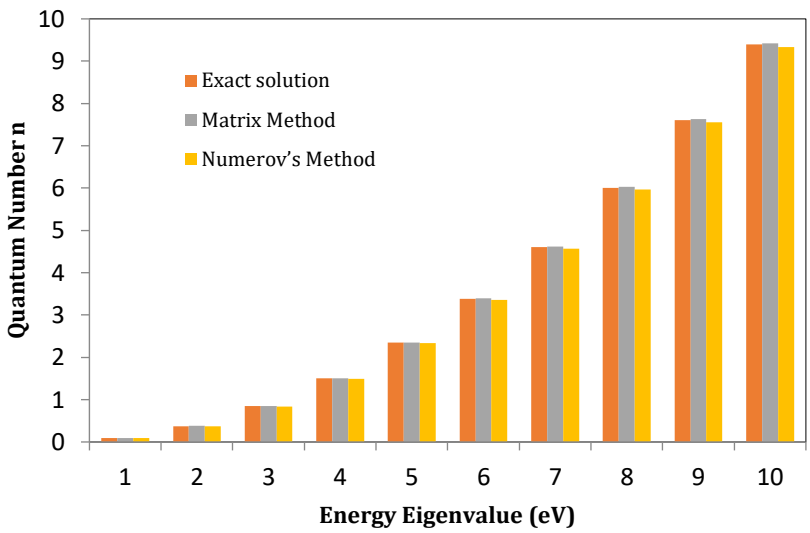


Fig. 3. A comparison of exact solution of energy eigenvalues for the first ten states for the infinite well with, width L=2 *nm* and number of points N=500, with the values obtained from Numerov and Matrix methods.

3. Conclusions

This paper is concerned with solving the Time-Independent Schrödinger Equation using numerical analysis. An attempt is made to find the energy eigenvalues and wave functions for the particle inside the infinite square well potential via the approximation methods; in particular Numerov and Matrix methods. The numerical results obtained are physically acceptable. The obtained results from both methods are in better agreement and very close to the exact solution results. However, the Matrix Method results are very close to the exact solution than those from the Numerov Method, the validity and accuracy of the two methods are demonstrated and the numerical simulations prove the advantages of the two methods. The merits of these numerical methods are to avoid a huge expense in time when solving Schrödinger equation. The accuracy and efficiency of this scheme may be also used to solve the Time-Dependent Schrödinger Equation.

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