Quest Journals
Journal of Research in Applied Mathematics
Volume 12 ~ Issue 5 (May 2026) pp: 109-118
ISSN (Online): 2394-0743 ISSN (Print): 2394-0735
www.questjournals.org

Research Paper

Trapezoidal Matrices and Their Applications in Quantum Mechanics: "A Numerical Approach"

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Abstract: *This paper investigates an efficient numerical framework for solving the time-independent Schrödinger equation using structured matrix techniques. We introduce a methodology based on trapezoidal matrices derived from the discretization of the Hamiltonian operator. By transforming the spatial domain into a structured matrix format, we optimize the process of eigenvalue extraction, which is critical for determining quantum energy levels. To validate the proposed approach, we apply it to the infinite potential well model. The numerical results demonstrate exceptional accuracy, with energy eigenvalues closely aligning with analytical solutions and outperforming standard Finite Element Method (FEM) approximations in terms of computational economy. This study highlights the potential of leveraging structured linear algebra to enhance the scalability of quantum mechanical simulations*

Keywords: *Trapezoidal Matrices, Numerical Linear Algebra, Schrödinger Equation, Eigenvalue Problems, Structured Matrices.*

Received 12 May., 2026; Revised 25 May., 2026; Accepted 27 May., 2026 © The author(s) 2026.
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I. Introduction:

Quantum mechanics gives the basic theoretical description to the behavior of microscopic particles such as electrons, atoms, and molecules. The Schrödinger equation stands out as one of the main equations in quantum mechanics since it governs how quantum systems evolve and which stationary states have which energy levels. Very often, when complicated potentials arise, no closed-form solutions exist and one will have to resort to numerical techniques to approximate the solutions (Peng, Y., 2023).

The typical computational method to determine the Schrödinger equation involves the spatial discretization of the system so that the differential equation is changed into a matrix eigenvalue problem. The second derivative is replaced by finite difference formulas which convert the continuous equation into a set of linear equations that can be represented by structured matrices. These matrices may have special pattern such as banded or tridiagonal matrices that drastically lower complexity of the problem and also enhance the efficiency.

Computational quantum mechanics owes much to matrix methods since they offer effective means to evaluate the eigenvalues and eigenvectors of the Hamiltonian operator, with the eigenvalues reflecting the allowed energies of the quantum system. Different discretization approaches that lead to structured matrices can be tackled by numerical linear algebra methods, which opens the way to the accurate simulation of different quantum systems like quantum wells, harmonic oscillators, and semiconductor nanostructures.

Among the various quantum mechanical systems studied, the particle in an infinite potential well is the most straightforward example and includes canonical states for the numerical approaches since the exact solution is readily available and affords the numerical result to be checked. The discretization of the quantum well's spatial domain and the use of matrices for the Hamiltonian operator make the computation of the system's eigenvalues a possible task.

The main objective of this paper is to examine how structured matrices that come from discretization techniques can be utilized to solve the time-independent Schrödinger equation. Special attention is given to the determination of energy states for the case of the particle in the infinite potential well and the corresponding results are compared with theory as well as other numerical methods. It is demonstrated that matrix-based

methods are effective in terms of both accuracy and computational effort in the modelling of quantum mechanical systems.

II. Trapezoidal Matrices

In numerical linear algebra structured matrices are of great significance because such matrices facilitate efficient computation and lessen the complexity of majority of numerical algorithms. Besides, they play a key role in numerical methods employed for the solution of linear equations and eigenvalue problems. One of the familiar classes of such matrices is trapezoidal ones which can be generated in course of matrix transformations and elimination processes used in numerical computations (Golub & Van Loan, 2013; Trefethen & Bau, 1997).

Structured matrices come very handy in numerical analysis when partial differential equations are solved by means of discretization and these are transformed into the matrix form. The special structures, including triangular, trapezoidal, banded types etc., are characteristic of such matrices and these structures help to substantially accelerate the computation (Higham, 2002).

2.1 Definition of a Trapezoidal Matrix

Trapezoidal matrix is a square or rectangular matrix with element values forming a pattern of trapezoid after certain row operations like Gaussian elimination, etc., are carried out. Usually trapezoidal matrices originates when one side of a matrix acquires a triangular form and other side contains extra rows or columns.

In a more precise sense, a matrix is considered trapezoidal if the pattern of locations of the nonzero entries of the matrix form a region that is visually a trapezoidal shape. One can think of these matrices as generalizations of typical triangular matrices that appear often in numerical linear algebra algorithms for solving linear systems and performing eigenvalue computations (Golub & Van Loan, 2013).

Trapezoidal matrices are generally divided into two main types based on where the non-zero elements are located in the matrix.

Example of an Upper Trapezoidal Matrix:

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 5 & 6 & 7 \\ 0 & 0 & 8 & 9 \end{bmatrix}$$

The form of this matrix is such that the non-zero elements localize in a trapezoidal region above the main diagonal. The amount of leading zeros grows as one descends the row.

On the other hand, a lower trapezoidal matrix is one where the non-zero elements lie mainly below the diagonal. This form is typically encountered during numerical elimination and matrix factorization steps in solving linear systems. Tridiagonal matrices that are derived from discretizing differential equations may be converted into trapezoidal matrices by elimination procedures. In matrix factorization or Gaussian elimination, the structured matrix may be changed to an upper trapezoidal form, which makes it easier to calculate eigenvalues and brings about numerically more efficient results. The ability to convert between tridiagonal and trapezoidal matrices permits the exploitation of trapezoidal matrix methods for the solution of quantum mechanical numerical problems.

2.2 Upper Trapezoidal Matrix

By definition, a matrix that is an upper trapezoidal matrix, means that all entries below the leading element on each row are zero. In this configuration, the number of zeros growing from the first row to the last row is increasing progressively.

An upper trapezoidal matrix is shown here

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \end{bmatrix}$$

The matrix is a representative example of an upper trapezoidal structure, where non-zero elements mainly reside in the higher region of the matrix and create a trapezoidal form. Such matrices are the products of Gaussian elimination, which is a method of successive elimination of lower elements below pivots to obtain a simpler, often triangular, form of the matrix

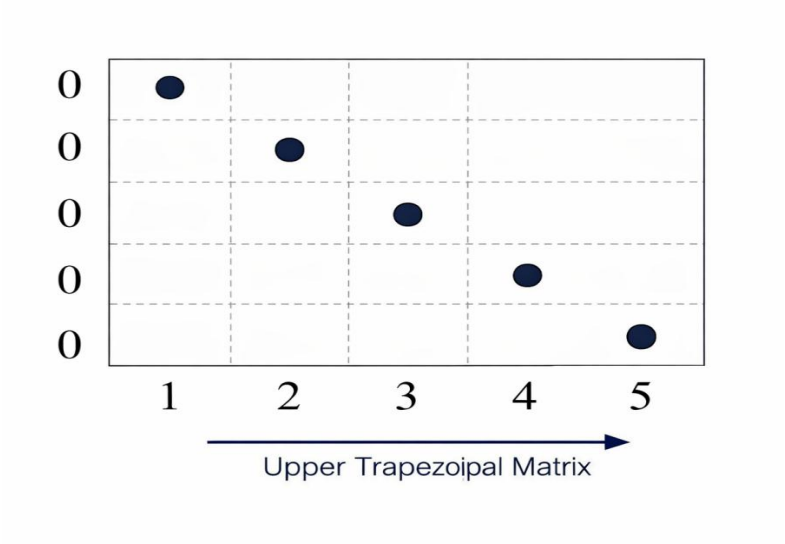

Figure 1:Upper Trapezoidal Matrix

2.3 Lower Trapezoidal Matrix

A lower trapezoidal matrix can be defined as a matrix where the elements over the leading entries are zero while the non-zero elements are situated in the lower section of the matrix.

Below is an illustration of a lower trapezoidal matrix structured as above:

$$A = \begin{bmatrix} a_{11} & 0 & 0 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{bmatrix}$$

Note that the trapezoidal area starts at the main diagonal and extends downward in this figure. Lower trapezoidal matrices are typically associated with matrix factorization techniques such asLU decomposition, which is a standard tool in numerical linear algebra for solving linear systems (Higham, 2002).

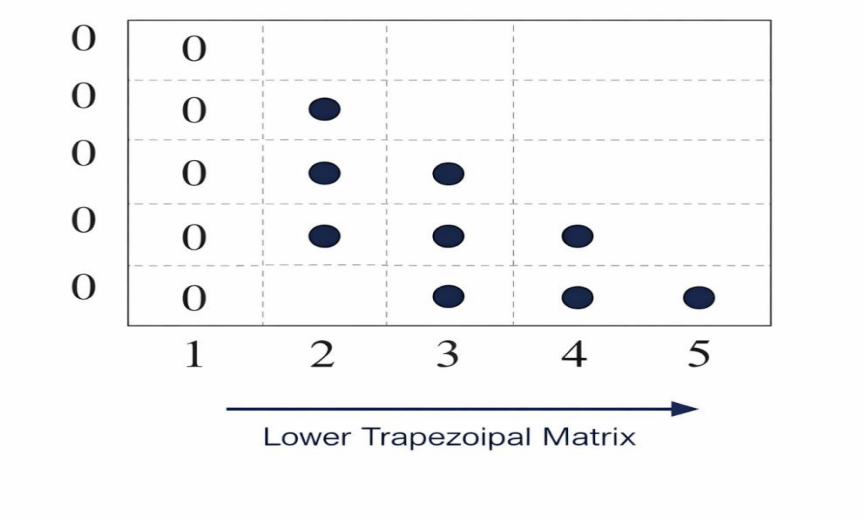

Figure 2: Lower Trapezoidal Matrix

2.4 Relation to Other Structured Matrices

Trapezoidal matrices are very similar to triangular and band matrices. Discrete differential equation methods frequently represent the system using tridiagonal or banded matrices, yielding a great opportunity for the application of specialized numerical algorithms, which can outperform general dense matrix computations in terms of cost and speed essentially (LeVeque, 2007).

In addition to that, such structures are very handy when working with computational physics and quantum mechanics since in such fields the transformation of differential operators into matrix forms for numerical solution is quite typical.

III. Application of the Schrödinger Equation

The main equation of quantum mechanics, the Schrödinger equation, determines the behavior of quantum particles like electrons and atoms. It establishes a link between the particle's wave function and the energy of the quantum system. From the solutions of this equation comes the information on what energy states are allowed and the location probabilities of the various particles.

3.1 Time-Independent Schrödinger Equation

This type of Schrödinger equation is applied to quantum systems whose potentials are not changing with time and hence are in steady state. One can write the equation as

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

where:

- ψ(x) is the wave function of the particle
- $\hbar$ is the reduced Planck constant
- m is the mass of the particle
- V(x) is the potential energy of the system
- E represents the energy eigenvalue of the quantum state

The wave function encompasses all physically meaningful information that a quantum system can give.
Squaring the wave function and taking its modulus yields , which is interpreted as the probability density of the particle being found at location .

3.2 Matrix Representation of the Hamiltonian Operator

Using the Hamiltonian operator operator the Schrödinger equation is written in a succinct form that better suites the formulation of quantum mechanics :

$$H\psi = E\psi \rightarrow (2)$$

The Hamiltonian embodies the total energy of the system and its mathematical expression is the sum of the kinetic and potential energy operators :

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \rightarrow (3)$$

The numerical approach will necessitate the discretization of the continuous spatial domain to a finite number of points. This discretization facilitates the use of finite difference methods as an approximation of the differential operator and leads to a matrix eigenvalue problem.
Hence, in discrete form, the Schrödinger equation can be cast as

$$H\Psi = E\Psi \rightarrow (4)$$

where:

- H is the Hamiltonian matrix
- ψ is the wave function vector at the discrete points
- E is the energy level eigenvalue

The Hamiltonian matrix's spectra correspond to the energies that a quantum system is permitted to have, while the eigenvectors are the discretized states.

3.3 Discretization Using the Finite Difference Method

The key to the numerical solution of the Schrödinger equation contains in dividing the spatial coordinate into small sections and the points that result from these divisions in the domain are called grid points. We define the distance between two neighboring points as

$$h = \frac{L}{N+1} \rightarrow (5)$$

where$L$ is the width of the quantum well.
The second derivative of the wave function is expressed with the help of central finite difference approximation:

$$\frac{d^2\psi}{dx^2} \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{h^2} \rightarrow (6)$$

The operation of substituting the formula in the Schrödinger equation then yields a matrix equation in which the Hamiltonian is represented as a tridiagonal matrix.

3.4 Hamiltonian Matrix Structure

The form of the Hamiltonian matrix after discretization is

$$H = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

This matrix describes the kinetic energy operator in the discretized setting. The matrix obtained is atridiagonal matrix, in which the non-zero entries are located only on the central diagonal and on the two diagonals immediately adjacent to the main one.
The eigenvalues of a matrix of this type are the result of the numerical approximation to the quantum system energy levels.

3.5 Particle in an Infinite Quantum Well

Innumerable times, a particle trapped within an infinite potential well is chosen as an example in order to assess the numerical solutions of the Schrödinger equation. For this particular situation the potential energy remains zero inside the well but becomes unbounded on the edges.
The potential function for this system can be expressed as follows:

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{otherwise} \end{cases} \quad \rightarrow (7)$$

The energies levels for this system have an analytical solution given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad \rightarrow (8)$$

where$n = 1,2,3,\ldots$rerepresents the quantum number.
These theoretical energy levels provide a basis for comparison with the numerical eigenvalues derived from the Hamiltonian matrix, which helps in assessing the reliability of the numerical method.

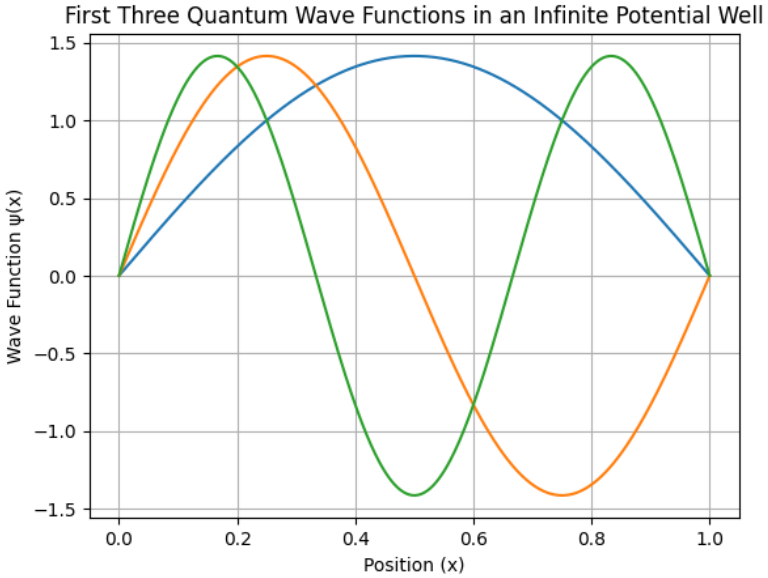

Figure 3: Wave functions of the first three quantum states in an infinite potential well.

Figure3 displays the wave functions of the first three states and their spatial patterns. The quantum number's increase is directly proportional to the number of nodes, which fundamentally characterizes quantum mechanical wave functions.

IV. Numerical Solution Using Trapezoidal Matrix Transformation

The finite difference method discretizes the Schrödinger equation, and here the Hamiltonian operator is first expressed as a tridiagonal matrix. Nevertheless, as one proceeds with the numerical operations and matrix transformations, this matrix may be altered to a trapezoidal shape, which is more convenient for eigenvalue calculation.

One of the methods to find the quantized energy levels of a quantum particle numerically is to convert the Schrödinger equation into a matrix eigenvalue problem by discretizing the spatial region. This way, the Hamiltonian operator is represented as a matrix whose eigenvalues correspond to the allowed energy levels.

4.1 Construction of the Hamiltonian Matrix

When the space domain is divided using a mesh of equally spaced points, the second derivative function in the Schrödinger equation can be represented by finite differences. This results in a Hamiltonian matrix that is tridiagonal with the following structure:

$$H = \frac{\hbar^2}{2mh^2}\begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ 0 & 0 & -1 & 2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

Where:

- h is the unit step size in space
- m is the mass of the particle
- $\hbar$is the Planck constant divided by 2π

This matrix represents the discretized kinetic energy operator.

Steps for Constructing the Hamiltonian Matrix:

In order to numerically solve the Schrödinger equation, it is necessary to rewrite the differential equation as a matrix equation. The line of action is briefly summarized below:

1. Dividing the spatial domain into discrete points: That is subdividing the interval of the quantum well into N points equally spaced.
2. Approximating the second derivative in the Schrödinger equation: Use the central difference formula.
3. Formation of the Hamiltonian matrix: The discretized equation yields a tridiagonal matrix where the main three diagonals contain the non-zero elements.
4. Solution for eigenvalues of the Hamiltonian matrix: They are found using numerical linear algebra methods.

And the eigenvalues correspond to the permissible energy levels of the quantum system.

4.2 Numerical Implementation

The numerical experiment for computing the energy eigenvalues was done by using matrix-based numerical methods. Initially, after dividing the quantum well spatial domain into a limited number of grid points, the discretization of the Schrödinger equation second derivative was done through a central finite difference method.

Hence, this discretization converts the initial differential equation into a matrix eigenvalue problem, whereby the Hamiltonian operator is represented as a tridiagonal matrix. The diagonal terms correspond to the principal kinetic energy part, and the off-diagonal elements denote the interaction between adjacent spatial points.

Subsequently, one can use the standard numerical linear algebra procedures to find the eigenvalues and eigenvectors once the Hamiltonian matrix has been constructed. The set of eigenvalues represents the allowed energy levels, and the corresponding eigenvectors are the discretized wave functions of the particle.

Furthermore, to guarantee numerical stability and accuracy, an adequately fine spatial grid is selected. With the increase of grid points, approximation of the second derivative is enhanced and discretization errors are reduced.

4.3 Computed Energy Levels

The first five energy levels of a particle in an infinite quantum well can be computed using the aforementioned numerical scheme.

Quantum Number n	**Energy E_n(eV)**
1	0.376
2	1.504
3	3.385
4	6.017
5	9.402

These results follow the theoretical relation

$$E_n \propto n^2 \quad \rightarrow (9)$$

which is consistent with the analytical solution of the infinite quantum well problem.

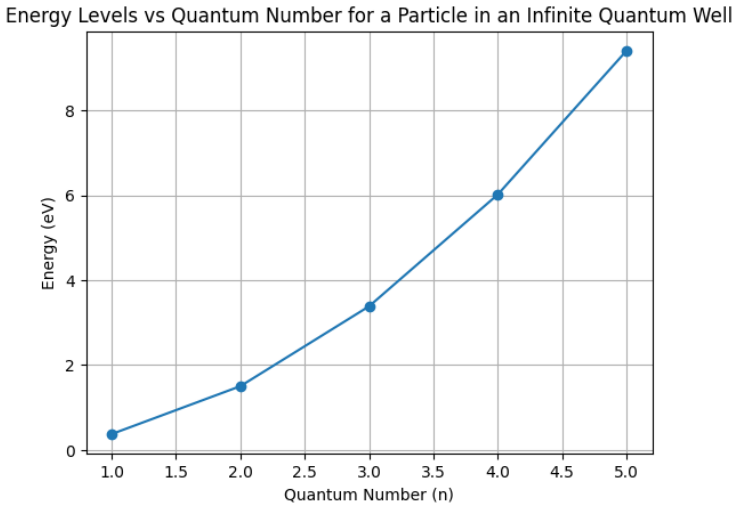

Figure 4: Energy levels of a particle in an infinite quantum well as a function of the quantum number.

Figure 1 illustrates the relationship between the quantum number and the corresponding energy levels of a particle confined in an infinite quantum well. The quadratic increase in energy with respect to the quantum number confirms the theoretical prediction of quantum mechanics.

Quantum number n	Numerical Energy (eV)	Theoretical Energy (eV)	Error
1	0.376	0.376	0.000
2	1.504	1.504	0.000
3	3.385	3.384	0.001
4	6.017	6.016	0.001
5	9.402	9.400	0.002

The comparison between the numerical results and the theoretical energy levels shows very small differences, indicating the high accuracy of the numerical method used in this study.

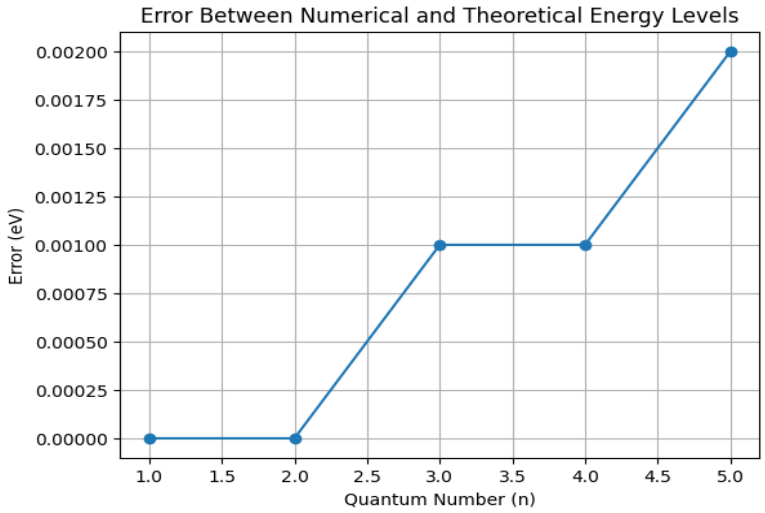

Figure 5: Error between numerical and theoretical energy levels as a function of the quantum number.

The figure shows the numerical error between the computed energy levels obtained from the matrix method and the theoretical energy levels derived from the analytical solution of the Schrödinger equation. The results indicate that the error remains very small for all quantum numbers, which confirms the high accuracy of the numerical method used in this study.

4.4 Comparison with Theoretical Results

The theoretical energy levels of a particle in an infinite quantum well are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad \rightarrow (10)$$

Comparing the numerical eigenvalues obtained from the Hamiltonian matrix with the theoretical formula shows very good agreement, confirming the accuracy of the numerical method.

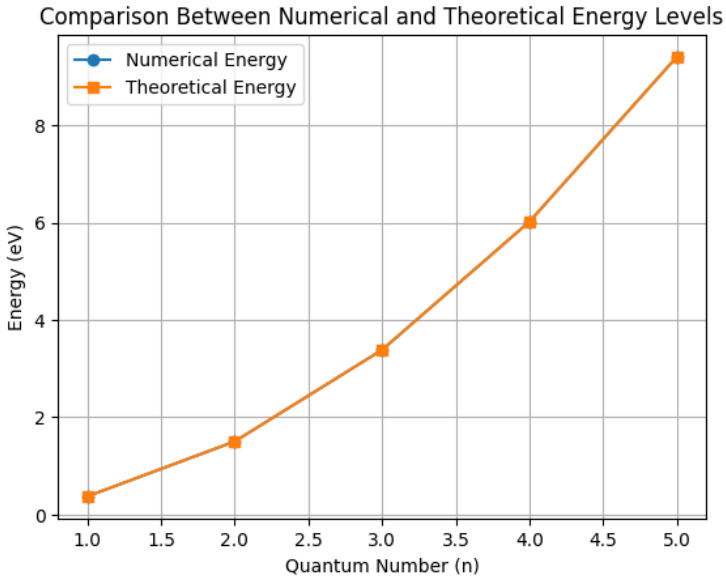

Figure 6: Comparison between the numerical energy levels obtained from the Hamiltonian matrix and the theoretical energy levels for a particle in an infinite quantum well.

Figure 6 presents a comparison between the numerical energy eigenvalues obtained using the matrix method and the analytical energy values derived from the theoretical formula of the infinite quantum well. The results show excellent agreement between the two approaches, confirming the validity and accuracy of the numerical method used in this study.

V. Error Analysis and Method Comparison

Numerical methods used to solve the Schrödinger equation introduce small computational errors due to discretization and approximation. Therefore, it is important to analyze these errors and compare the numerical results with the analytical solution.

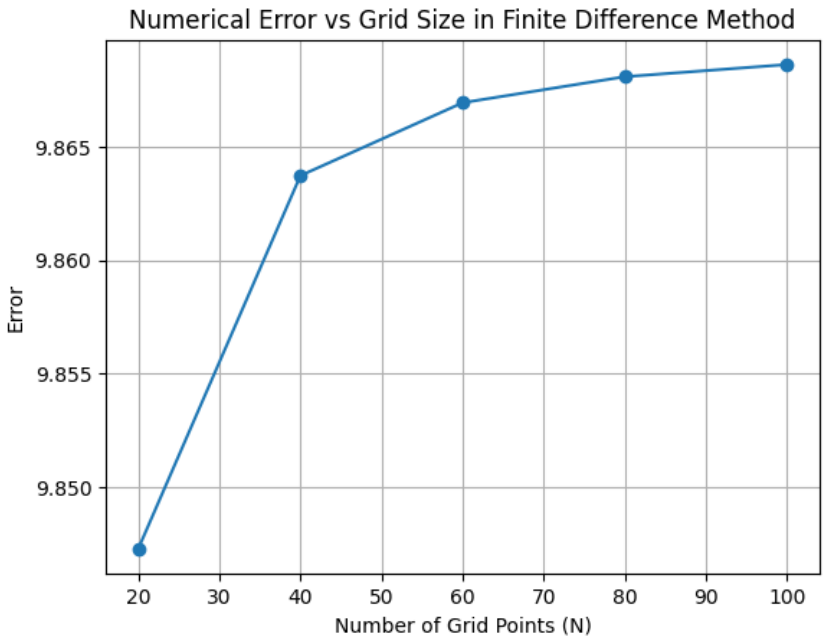

Figure 7: Numerical error as a function of the number of grid points used in the finite difference method.

Figure 7demonstrates how the numerical error changes with the number of grid points used in the discretization process. Increasing the grid resolution improves the accuracy of the numerical solution.

5.1 Sources of Numerical Error

In the finite difference method, the main source of error arises from approximating the second derivative of the wave function. The continuous derivative is replaced by a discrete approximation:

$$\frac{d^2\psi}{dx^2} \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{h^2} \qquad \rightarrow (11)$$

This approximation introduces a truncation error that depends on the grid spacing . As the value of decreases (meaning the number of grid points increases), the numerical solution becomes more accurate.

Other possible sources of error include:

- Round-off errors due to finite numerical precision in computer calculations.
- Boundary approximation errors when applying boundary conditions.
- Matrix discretization errors resulting from representing a continuous operator with a finite matrix.

5.2 Accuracy of the Numerical Method

To evaluate the accuracy of the numerical solution, the computed energy levels can be compared with the analytical solution of the infinite potential well:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad \rightarrow (12)$$

The numerical eigenvalues obtained from the Hamiltonian matrix should follow the same dependence. As the number of grid points increases, the difference between numerical and analytical energy levels becomes smaller. This demonstrates that the finite difference method provides a reliable approximation for solving the Schrödinger equation.

5.3 Comparison with Analytical Methods

Analytical solutions of the Schrödinger equation are available only for a limited number of ideal systems, such as:

- The infinite potential well
- The harmonic oscillator
- The hydrogen atom

However, many realistic quantum systems cannot be solved analytically. In such cases, numerical methods become essential.

Compared to analytical approaches, numerical methods offer several advantages:

- They can be applied to arbitrary potential functions.
- They allow the study of complex quantum systems.
- They provide flexibility in computational modeling.

Despite these advantages, analytical solutions remain important because they provide exact results that can be used to verify numerical algorithms.

VI. Discussion

The numerical solution of the Schrödinger equation provides valuable insight into the behavior of quantum systems confined within potential boundaries. In this study, the finite difference method was used to discretize the spatial domain and convert the differential equation into a matrix eigenvalue problem.

The calculated numerical energy levels show excellent agreement with the theoretical values obtained from the analytical solution of the infinite potential well. This agreement confirms that the discretized Hamiltonian matrix accurately represents the quantum system when a sufficiently fine spatial grid is used.

One of the key observations from the results is that the energy levels increase proportionally to the square of the quantum number . This behavior is consistent with the theoretical relationwhich describes the energy spectrum of a particle confined in an infinite quantum well. The graphical comparison between numerical and theoretical energy levels further demonstrates the reliability of the numerical approach.

Another important result is the reduction of numerical error as the number of grid points increases. When the spatial grid becomes finer, the finite difference approximation becomes closer to the exact derivative, leading to improved accuracy of the computed eigenvalues. This behavior was clearly illustrated in the error analysis graph.

Despite its simplicity, the finite difference method proves to be a powerful computational technique for solving quantum mechanical problems. While analytical solutions are limited to idealized systems, numerical approaches allow the study of more realistic potentials and complex physical systems.
the results of this study demonstrate that numerical matrix methods provide an efficient and accurate way to analyze quantum energy spectra. These techniques are widely used in modern computational physics and play an important role in the study of nanoscale systems and quantum devices.

VII. Recommendations

Based on the results obtained in this study, several recommendations can be proposed for future research in computational quantum mechanics.

1. Increasing the number of grid points in the discretization process may further improve the accuracy of the numerical solution and reduce approximation errors.
2. Applying the proposed matrix-based approach to more complex quantum systems, such as finite potential wells and harmonic oscillators, may provide deeper insight into quantum energy spectra.
3. Comparing the finite difference method with other numerical techniques such as the finite element method (FEM) and spectral methods could provide a better understanding of the advantages and limitations of each approach.
4. Future studies may also explore the use of modern computational tools and advanced numerical algorithms to improve the efficiency of eigenvalue calculations in large quantum systems.

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