Computational Analysis of the Time-Independent Schrödinger Equation: A Numerical Approach

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1 Introduction and Theoretical Background

Quantum mechanics, a foundational theory in physics developed in the early 20th century, governs the behavior of matter and energy at microscopic scales. It introduces principles such as wave-particle duality, the quantization of energy, and the uncertainty principle. One key aspect involves the concept of energy levels, where the energy of quantum systems is quantized into discrete values. This quantization is fundamental to understanding phenomena at the atomic and subatomic levels.

In this computational physics project, we delve into the simulation of energy levels within finite and infinite quantum wells and harmonic oscillators. By solving the Schrödinger equation, we aim to unveil the discrete energy states associated with these systems, shedding light on the intricate behavior of particles in confined spaces and under harmonic forces.

1.1 Schrödinger Equation and Hamiltonian Formulation

The time-independent Schrödinger equation is a fundamental equation in quantum mechanics that describes how the quantum state of a physical system changes in time. It is given by:

$$\hat{H}\psi = E\psi \tag{1}$$

where $\hat{H}$ is the Hamiltonian operator, ψ is the wave function, and E is the energy eigenvalue. This equation states that the Hamiltonian operator acting on the wave function ψ yields the energy eigenvalue E multiplied by the wave function ψ.

1.1.1 Hamiltonian Operator

The Hamiltonian operator $(\hat{H})$ represents the total energy of the system and is formulated as the sum of kinetic energy (T) and potential energy (V):

$$\hat{H} = \hat{T} + \hat{V} \tag{2}$$

The kinetic energy operator $(\hat{T})$ in quantum mechanics is associated with the motion of the particle. For a particle moving in one dimension, it can be expressed as:

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{3}$$

where $\hbar$ is the reduced Planck constant, m is the mass of the particle, and $\frac{\partial^2}{\partial x^2}$ is the second derivative with respect to position. This operator reflects the quantum mechanical version of the classical kinetic energy.

The potential energy operator ($\hat{V}$) depends on the specific potential energy function $V(x)$ of the system. For a particle in a potential well, $V(x)$ is defined by the shape of the well. In the case of an infinite or finite quantum well, $V(x)$ is piecewise defined. The potential energy operator is diagonal in the position representation, meaning it acts multiplicatively on the wave function:

$$\hat{V}\psi(x) = V(x)\psi(x) \tag{4}$$

Then, to find the allowed energy levels and corresponding wave functions of a quantum system, one must solve the time-independent Schrödinger equation with the appropriate Hamiltonian. This involves substituting the expressions for $\hat{T}$ and $\hat{V}$ into the Hamiltonian and solving the resulting differential equation under the given boundary conditions and constraints of the system.

1.2 Quantum Wells

In the realm of quantum mechanics, finite and infinite quantum wells represent distinct scenarios of particle confinement, particularly for electrons. The potential energy profiles associated with these wells contribute to the quantization of energy levels within the systems.

1.2.1 Infinite Quantum Well

An infinite quantum well is a theoretical construct modeling a system with an infinite potential barrier outside the defined boundaries. The potential energy profile for an infinite quantum well is given by:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a \\ \infty & \text{otherwise} \end{cases} \tag{5}$$

In this case, the particle is confined within the well ($0 < x < a$) due to the infinite potential outside the well. Similar to the finite well, the particle experiences quantized energy levels within the well.
The quantized energy levels in the infinite quantum well are described by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{6}$$

where n is the quantum number (1, 2, 3, ...), $\hbar$ is the reduced Planck constant, and m is the mass of the particle, And the corresponding wavefunctions are:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{7}$$

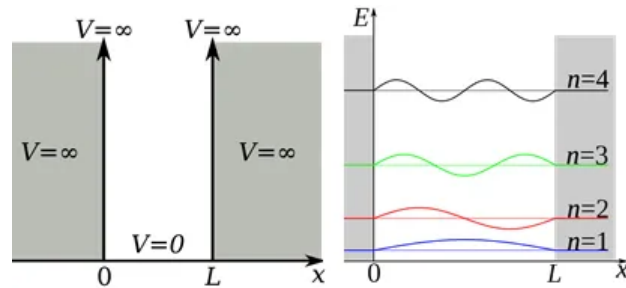for $0 < x < a$, and $\psi_n(x) = 0$ for $x \leq 0$ or $x \geq a$.

Figure 1: Graph showing the infinite potential well and the expected wavefunctions for different quantum numbers n.

1.2.2 Finite Quantum Well

A finite quantum well is a potential well with finite depth, used to model quantum systems where a particle is confined within a region of space bounded by potential barriers of finite height. This model is crucial for understanding various quantum phenomena, including quantum tunneling.

The potential energy profile for a finite quantum well is defined as:

$$V(x) = \begin{cases} V_0 & \text{for } x < 0 \text{ or } x > a \\ 0 & \text{for } 0 \leq x \leq a \end{cases} \tag{8}$$

where V_0 is the height of the potential barriers and a is the width of the well. The boundary conditions for the finite quantum well are set by the continuity of the wavefunction and its derivative at the boundaries of the well, $x = 0$ and $x = a$.

The time-independent Schrödinger equation for a particle of mass m in this potential is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{9}$$

To solve this equation, one typically divides the problem into three regions: $x < 0$, $0 \leq x \leq a$, and $x > a$, and solves the equation in each region subject to the appropriate boundary conditions. The solutions in the barrier regions ($x < 0$ and $x > a$) often involve exponential decay or growth, reflecting the quantum tunneling effect. In the well region ($0 \leq x \leq a$), the solutions are sinusoidal. Matching these solutions and their derivatives at the boundaries leads to a transcendental equation, which is usually solved numerically to find the allowed energy levels E and corresponding wavefunctions ψ. We denote that an analytical solution example will be presented through the next few sections.

1.3 Harmonic Oscillators

Harmonic oscillators play a crucial role in quantum mechanics, representing systems where particles undergo periodic motion around an equilibrium position. In the quantum realm, the harmonic oscillator model is commonly employed to describe phenomena such as molecular vibrations, atomic bonds, and vibrational modes in solid-state physics.

1.3.1 Harmonic Oscillator Potential Energy Function

The potential energy function ($V(x)$) for a harmonic oscillator is characterized by a quadratic dependence on the displacement (x) from the equilibrium position. In one dimension, the potential energy function is given by:

$$V(x) = \frac{1}{2}kx^2 \tag{10}$$

Here, k is the force constant or spring constant, representing the stiffness of the oscillator. The variable x represents the displacement from the equilibrium position. The quadratic form of the potential energy function reflects the restoring force exerted by the oscillator, which is proportional to its displacement. This form of the potential leads to simple harmonic motion in classical mechanics and plays a central role in quantum mechanics for modeling vibrational motion.

1.3.2   Quantization of Energy Levels

In quantum mechanics, the quantization of energy levels for a harmonic oscillator arises as a fundamental consequence of solving the Schrödinger equation with the harmonic oscillator potential. The solutions to the Schrödinger equation reveal discrete energy eigenvalues given by:

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega \tag{11}$$

where n is a non-negative integer representing the quantum number, $\hbar$ is the reduced Planck constant, and ω is the angular frequency of the harmonic oscillator. The angular frequency ω is related to the force constant k and the mass m of the oscillator by $\omega = \sqrt{\frac{k}{m}}$. These quantized energy levels indicate that the harmonic oscillator can only possess certain discrete energy values, a fundamental departure from classical mechanics where the energy can take any continuous value.
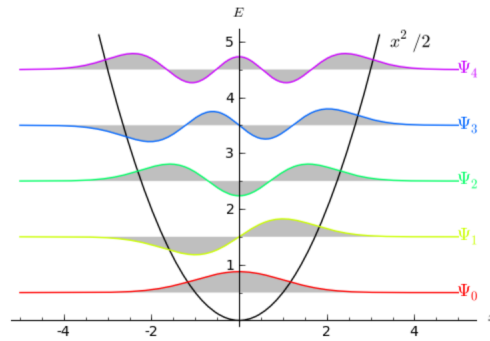

Figure 2: Graph showing the harmonic oscillator (quadratic potential) and the expected wavefunctions$n$.

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2 Numerical Methods

2.1 Finite Difference Method

The finite difference method is a numerical technique that can be used to find the solution of differential equations with defined boundary conditions. It utilizes finite difference formulas[1] applied at uniformly distributed grid points to approximate the derivatives in the differential equation, transforming a differential equation into a system of algebraic equations.

We can divide the the interval of $[a,b]$ into n equal subintervals of length h as shown in the figure below. The value of the solution at these discrete points is approximated by solving algebraic equations containing finite differences and values from nearby points.
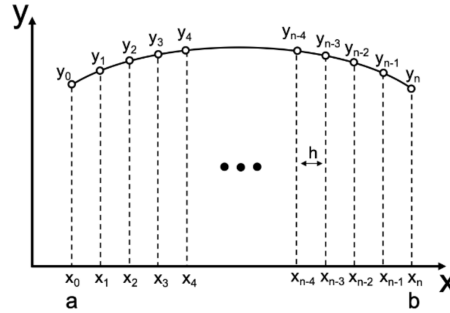
The central difference formulas are preferred in finite difference method for they tend to offer higher accuracy in approximating derivatives as compared to other formulas

2.1.1 Finite Difference Method for the Schrödinger equation

The time-independent Schrodinger equation is a linear ordinary differential equation that describes the state function of a quantum-mechanical system. Particle variables such as momentum and energy can take many different values; for each value of said variables, there exists a wave function that describes the state of the particle. The solution of the Schrodinger equation yields quantized energy levels as well as wavefunctions of a given quantum system.

Consider a particle in the spatial domain x $\in [a, b]$, we can divide this domain intro n discrete points, each point denoted by $x_0, x_1, x_2, ..., x_{n-1}$ where $x_0 = a$ and $x_n = b$. The wavefunction $\psi(x)$ at each point will be denoted as $\psi_0, \psi_1, \psi_2, ..., \psi_{n-1}$. The step difference is given by $\Delta x = \frac{b-a}{n}$. Time-independent Schrödinger equation for a one-dimensional quantum system is given as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{12}$$

Using the second-order central difference formula:

$$\frac{d^2y}{dx^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} \tag{13}$$

we can discretize the above equations, giving:

$$-\frac{\hbar^2}{2m}\frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{\Delta x^2} + V_i(x)\psi_i(x) = E\psi_i(x) \tag{14}$$

The above equation is a "discretized" form of Schrödinger equation.

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[1] https://lcn.people.uic.edu/classes/che205s17/docs/che205s17_reading_01e.pdf

2.2 Matrix Diagonalization

Matrix diagonalization is a technique used to transform a square matrix into a diagonal matrix through a similarity transformation. Essentially, it involves finding a set of eigenvectors and eigenvalues that allow you to express the matrix in a simpler form. It is important to note that not all matrices are diagonalizable. The diagonalizable matrices are those that have no defective eigenvalues (i.e., eigenvalues whose geometric multiplicity is less than their algebraic multiplicity).

2.2.1 Similarity Transformations

Two square matrices A and B are said to be similar if there exists an invertible $n \times n$ matrix P such that

$$B = P^{-1}AP \tag{15}$$

If two matrices are similar, then they have the same rank, trace, determinant and eigenvalues.

2.2.2 Formal Definition

Matrix A is diagonalizable, if there exists an invertible matrix P such that

$$D = P^{-1}AP \tag{16}$$

where D is a diagonal matrix, that is, a matrix whose non-diagonal entries are zero.

2.2.3 Relation To Eigenvalues and Eigenvectors

If we multiply both sides of the previous expression with the matrix P from the left, we can re-write the previous expression as

$$AP = PD \tag{17}$$

The kth column of AP can be expressed as AP_k, and the kth column of PD can also be expressed as PD_k, where D_k and P_k are the kth columns of D and P respectively.

We can see that PD_k is nothing more than a multiplication of the columns of matrix P with the values of the vector D_k, in other words, it is linear combination of the columns of P with coefficients taken from the vector D_k.

Since D is a diagonal matrix, the only non-zero entry of D_k is D_{kk}. Therefore,

$$PD_{kk} = D_{kk}P_k \tag{18}$$

We conclude that:

$$AP_k = D_{kk}P_k \tag{19}$$

The latter equality means that P_{kk} is an eigenvector of A associated to the eigenvalue D_{kk}.

2.2.4 Diagonalizing a Matrix

Let A be the $n \times n$ matrix that you want to diagonalize, assuming it is diagonalizable. The process of diagonalizing a matrix involves several steps. First, find the characteristic polynomial $p(t)$ of A. Then, determine the eigenvalues λ of the matrix A and their algebraic multiplicities from the characteristic polynomial $p(t)$. For each eigenvalue λ of A, find a basis of the eigenspace E_λ. If there is an eigenvalue λ such that the geometric multiplicity of λ, $\dim(E_\lambda)$, is less than the algebraic multiplicity of λ, then the matrix A is not diagonalizable. If this is not the case, and A is diagonalizable, proceed to the next step. Combine all basis vectors for all eigenspaces to obtain n linearly independent eigenvectors $v_1, v_2, v_3, \ldots, v_n$. Define the nonsingular matrix $P = [v_1, v_2, v_3, \ldots, v_n]$. Next, define the diagonal matrix D, whose (i, i)-entry is the eigenvalue λ corresponding to the eigenspace E_λ in which the ith column vector v_i is located. Finally, the matrix A is diagonalized as $D = P^{-1}AP$.

2.2.5 Matrix Diagonalization and Solving the Schrödinger Equation

When dealing with time-independent systems, solving Schrödinger's equation involves finding the eigenvalues and eigenvectors of the Hamiltonian operator. This leads to a matrix representation of the operator, and diagonalizing this matrix helps find the energy eigenvalues and corresponding eigenstates of the system.
The eigenvalues obtained from diagonalizing the Hamiltonian operator correspond to the allowed energy levels of the quantum system, while the eigenvectors represent the associated quantum states.
From the discretized equation in section 2.1.1, we can construct a matrix for each expression in the equation.

The kinetic energy matrix would be:

$$T = -\frac{\hbar^2}{2m(\delta x)^2} \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \tag{20}$$

The potential energy matrix:

$$V = \begin{bmatrix} V_1 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 \\ 0 & 0 & V_3 & 0 \\ 0 & 0 & 0 & V_4 \end{bmatrix} \tag{21}$$

Construct the Hamiltonian matrix:

$$H = T + V \tag{22}$$

Diagonalizing the Hamiltonian matrix, H, equips us with the eigenvalues (energies) and eigenvectors (wavefunctions).

3 Code Implementation

In this section, we provide a detailed explanation of the key components of a MATLAB implememntation we used to solve our problem. `schrodingerSolver`, designed to solve the Schrödinger equation for various potential profiles. The function allows users to choose between different potentials and calculates the corresponding eigenenergies and eigenfunctions, with the full working code provided in the Appendix.

3.1 Code Decomposition and Explanation

3.1.1 Initialization and User Inputs

The function begins by defining fundamental constants and then prompts the user for inputs to specify the potential type, dimensions of the well, effective mass of the particle, and other parameters.

```
% Constants
hbar = 1.0545718e-34; % Reduced Planck's constant (J s)
e = 1.60217662e-19;   % Elementary charge (C)
me = 9.10938356e-30 ;  % Electron mass (kg)

% User inputs
V_type = input('Enter your choice (1/2/3): ');
L_nm = input('Enter the width of the well in nm: ');
m_eff = input('Enter the effective mass of the particle: ');
N = input('Enter the number of grid points: ');
numEigenvaluesToPlot = input('Enter the number of eigenenergies to plot: ');
```

3.1.2 Potential Profile Setup

Based on the user's choice, the potential V is set up accordingly. For an infinite square well, the potential is zero inside the well and infinite outside. For a finite square well, it has a finite height specified by the user. For a harmonic oscillator, the potential is parabolic.

```
% Initialize the potential V for each type of well
V = zeros(N, 1);
V_inf = 1e9 * e;

if V_type == 1 % Infinite Square Well
    ...
elseif V_type == 2 % Finite Square Well
    ...
elseif V_type == 3 % Harmonic Oscillator
    ...
end
```

3.1.3 Hamiltonian Matrix Construction

The Hamiltonian matrix is constructed using the finite difference method. The main diagonal represents the potential energy at each point, and the off-diagonals represent the kinetic energy.

```
% Construct the Hamiltonian matrix H
t0 = hbar^2 / (2 * m * dx^2); % Kinetic energy coefficient
main_diag = 2 * t0 + V; % Main diagonal
off_diag = -t0 * ones(N-1, 1); % Off-diagonal
H = diag(main_diag) + diag(off_diag, 1) + diag(off_diag, -1);
```

3.1.4 Eigenvalue Problem and Plotting

The eigenvalue problem is solved using MATLAB's `eig` function. The eigenvalues represent the energy levels, and the eigenvectors are the corresponding wavefunctions. These are then plotted to visualize the results.

```
% Solve the eigenvalue problem
[psi, E] = eig(H);
energies_eV = diag(E) / e; % Convert energies to eV

% Plotting eigenenergies and eigenfunctions
...
```

4 Results and Validation

4.1 Infinite Square Well

For the infinite square well, the potential inside the well is zero, and it is infinite outside. The eigenenergies and eigenfunctions calculated by the 'schrodingerSolver' function for this potential were compared with the theoretical values. The energy levels for an infinite square well are given by the formula $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$, where n is the quantum number. The calculated eigenenergies matched closely with these theoretical values, validating the accuracy of the implementation.

4.1.1 Energy Comparison

The following table compares the exact theoretical energies with those calculated by the 'schrodingerSolver' function for the infinite square well: Specifications for the Infinite Square Well:

Quantum Number n	Theoretical Energy (eV)	Calculated Energy (eV)	Error (%)
1	0.0015	0.0015	0.00
2	0.0060	0.0060	0.00
3	0.0135	0.0135	0.00
4	0.0241	0.0240	0.04
5	0.0376	0.0376	0.00
6	0.0541	0.0541	0.00
7	0.0737	0.0736	0.14
8	0.0963	0.0962	0.10
9	0.1218	0.1217	0.08
10	0.1504	0.1503	0.07
11	0.1820	0.1819	0.05
12	0.2166	0.2164	0.09
13	0.2542	0.2540	0.08
14	0.2948	0.2946	0.07
15	0.3384	0.3382	0.06

Table 1: Comparison of theoretical and calculated energies for the Infinite Square Well with L = 5nm, n = 5000 points , and m = 1 m_e.

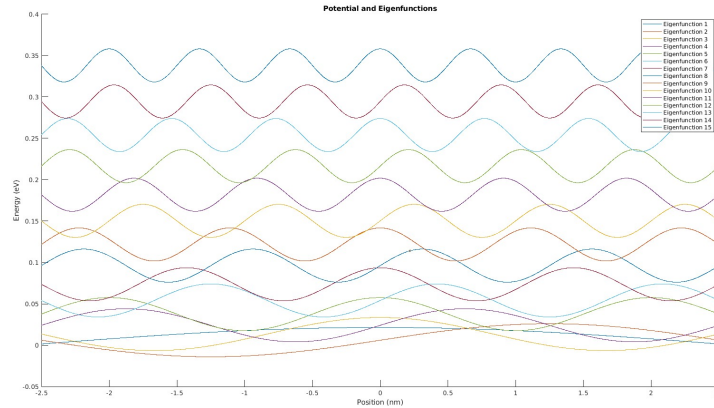Figure 3: Numerical eigenfunctions for the infinite Square Well with L = 5nm, n = 5000 points , and m = 1 m_e

4.2 Finite Square Well

In the case of the finite square well, the potential has a finite height specified by the user. The eigenenergies for this potential depend on the well's depth and width. The results obtained from the 'schrodingerSolver' function showed good agreement with the expected theoretical trends which were calculated analytically in a study available here[1].

Quantum Number n	Theoretical Energy (eV)	Calculated Energy (eV)	Error (%)
1	1.123	1.0735	4.40
2	4.461	4.2941	3.74
3	9.905	9.6616	2.46
4	17.162	17.1762	0.08

Table 2: Comparison of theoretical and calculated energies for the finite Square Well with L = 0.5nm, n = 5000 points , and m = .14 m_e

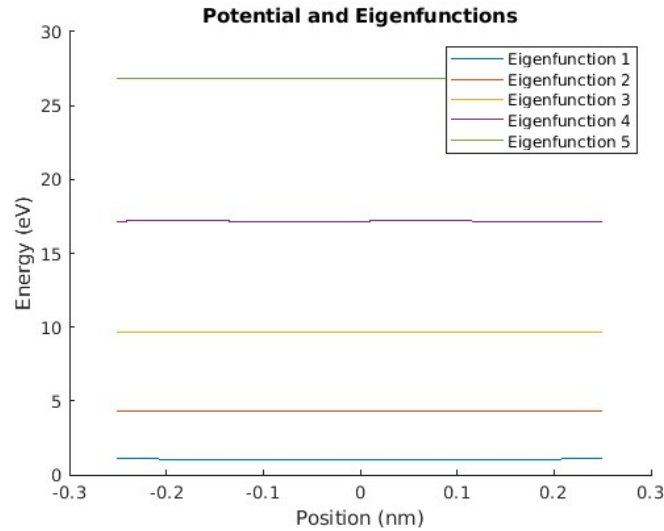Figure 4: Eigenenergies and eigenfunctions for the Finite Square Well with L = 0.5nm, n = 5000 points , and m = .14 m_e

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[1]See: http://ursula.chem.yale.edu/~batista/classes/vvv/FiniteSquareWell.pdf for an analytical approach to the finite square well problem.

4.3   Harmonic Oscillator

For the harmonic oscillator potential, the function calculates the eigenenergies and eigenfunctions for a parabolic potential. The theoretical energy levels for a quantum harmonic oscillator are given by $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. The results from the MATLAB implementation were consistent with these theoretical predictions, demonstrating the correct parabolic shape for the potential and the expected spacing between the energy levels.

4.3.1   Energy Comparison

The table below compares the exact theoretical energies with the calculated values for the harmonic oscillator:

Quantum Number n	Theoretical Energy (eV)	Calculated Energy (eV)	Error (%)
1	0.0239	0.0239	0.00
2	0.0717	0.0717	0.00
3	0.1195	0.1195	0.00
4	0.1673	0.1673	0.00
5	0.2152	0.2152	0.00
6	0.2630	0.2630	0.00
7	0.3108	0.3108	0.00
8	0.3586	0.3586	0.00
9	0.4064	0.4064	0.00
10	0.4542	0.4542	0.00
11	0.5020	0.5020	0.00
12	0.5498	0.5498	0.00
13	0.5977	0.5977	0.00
14	0.6455	0.6456	0.02
15	0.6933	0.6936	0.04

Table 3: Comparison of theoretical and calculated energies for the Harmonic Oscillator with width = 5nm, k= 0.3 eV/nm^2, m = 1 m_e, and n = 5000 points
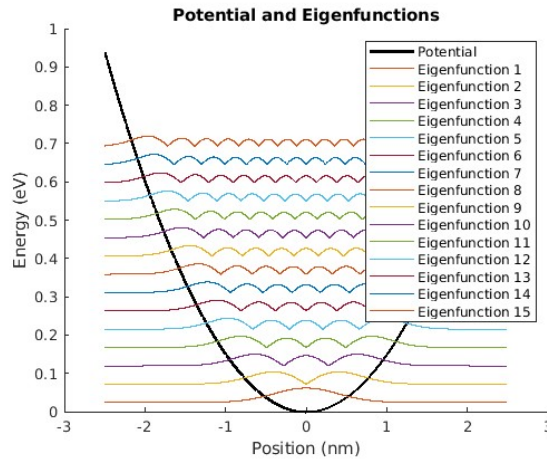

Figure 5: Numerical eigenfunctions for the Harmonic Oscillator with width = 5nm, k= 0.3 eV/nm^2, m = 1 m_e, and n = 5000 points.

5   Conclusion

The 'schrodingerSolver' function, implemented using the finite difference method, has demonstrated remarkable accuracy in calculating the eigenenergies for various quantum mechanical potentials. In the cases of the infinite square well and the harmonic oscillator, the errors were predominantly around 0.01 percent, underscoring the precision and reliability of the method in these scenarios. Even in the more complex case of the finite square well, where the highest observed error was 4.4 percent, the results still showed good agreement with the expected theoretical trends. This slight increase in error can be attributed to the inherent challenges in numerically approximating a system with finite boundaries, where the potential sharply changes.

Overall, the finite difference method has proven to be an absolutely successful and robust approach for solving the Schrödinger equation in various potential scenarios. Its ability to yield highly accurate results, especially in the infinite and harmonic oscillator cases, makes it a valuable tool in the study and understanding of quantum mechanical systems. The slightly higher error in the finite square well case also provides insightful learning opportunities, highlighting areas for further refinement and exploration in computational quantum mechanics.

References

[1] David J. Griffiths, *Introduction to Quantum Mechanics*, 2nd Edition, Pearson Education, 2004.

[2] H. M. Antia, *Numerical Methods for Scientists and Engineers*, 3rd Edition, Birkhäuser, 2012.

[3] Avtar S. Sehra, *Finite Element Analysis of the Schroedinger Equation*, 2007, `http://arxiv.org/abs/0704.3240v1`.

[4] Georgios E. Zouraris, *A linear implicit finite difference discretization of the Schrodinger-Hirota Equation*, 2017, `http://arxiv.org/abs/1706.03871v1`.

[5] M. Mangin-Brinet, J. Carbonell, C. Gignoux, *Exact boundary conditions at finite distance for the time-dependent Schrodinger equation*, 1998, `http://arxiv.org/abs/quant-ph/9804030v1`.

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[8] *Quantum Mechanics and Quantum Computation*, University of Illinois at Chicago, `https://lcn.people.uic.edu/classes/che205s17/docs/che205s17_reading_01e.pdf`.

[9] *Finite Square Well*, Yale University, `http://ursula.chem.yale.edu/~batista/classes/vvv/FiniteSquareWell.pdf`.

A   Schrodinger Solver Code

```matlab
function schrodingerSolver()
    % Constants
    hbar = 1.0545718e-34; % Reduced Planck's constant (J s)
    e = 1.60217662e-19;   % Elementary charge (C)
    me = 9.10938356e-30 ;  % Electron mass (kg)

    % User inputs in standard units
    disp('Select the potential type:');
    disp('1. Infinite Square Well');
    disp('2. Finite Square Well');
    disp('3. Harmonic Oscillator');
    V_type = input('Enter your choice (1/2/3): ');
    L_nm = input('Enter the width of the well in nm: '); % Width in nanometers
    L = L_nm * 1e-9; % Convert nm to m for calculations
    m_eff = input('Enter the effective mass of the particle as a ratio to me (electron mass)
    : '); % Effective mass as a ratio of electron mass
    m = m_eff * me; % Effective mass in kg
    N = input('Enter the number of grid points: ');
    numEigenvaluesToPlot = input('Enter the number of eigenenergies to plot: ');

    % Define spatial grid
    x = linspace(-L/2, L/2, N)'; % x goes from -L to L to center the harmonic oscillator
    dx = x(2) - x(1); % Grid spacing

    % Initialize the potential V for each type of well
    V = zeros(N, 1);
    V_inf = 1e9 * e;

    %theoritical energies from the analytic formula
    theoreticalEnergies = zeros(numEigenvaluesToPlot, 1);


    if V_type == 1 % Infinite Square Well
        V0_eV=V_inf;
        V(:) = 0;
        V(1) = V0_eV * e; % Set the first and last point to the barrier height
        V(end) = V0_eV * e;
    elseif V_type == 2 % Finite Square Well
        V0_eV = input('Enter the height of the finite well in eV: ');  % Height in electron
    volts
        V(1) = V0_eV * e;
        V(end) = V0_eV * e;
    elseif V_type == 3 % Harmonic Oscillator
        k_eV_per_nm2 = input('Enter the spring constant for the harmonic oscillator in eV/nm
    ^2: '); % Spring constant in eV/nm^2
        k = k_eV_per_nm2 * e * (1e9)^2; % Convert eV/nm^2 to J/m^2 for calculations
        V = 0.5 * k * (x).^2; % Parabolic potential centered at L/2
    end

    % Construct the Hamiltonian matrix H using finite differences
    t0 = hbar^2 /    (2 * m * dx^2); % Kinetic energy coefficient
    main_diag = 2 * t0 + V; % Main diagonal with kinetic and potential energy
    off_diag = -t0 * ones(N-1, 1); % Off-diagonal with kinetic energy
    H = diag(main_diag) + diag(off_diag, 1) + diag(off_diag, -1);

    % Solve the eigenvalue problem to find energy levels and wavefunctions
    [psi, E] = eig(H);
    energies_eV = diag(E) / e; % Convert the energies from J to eV for output

    % Calculate theoretical energies for Infinite Square Well and Harmonic Oscillator
    if V_type == 1 % Infinite Square Well
        for n = 1:numEigenvaluesToPlot
            theoreticalEnergies(n) = (n^2 * pi^2 * hbar^2) / (2 * m * L^2) / e; % Convert to
```

```matlab
        eV
63          end
64      elseif V_type == 3 % Harmonic Oscillator
65          omega = sqrt(k / m); % Angular frequency
66          for n = 1:numEigenvaluesToPlot
67              theoreticalEnergies(n) = (n - 0.5) * hbar * omega / e; % Convert to eV
68          end
69      end
70
71      % Plot the eigenenergies
72      figure;
73      hold on;
74      title('Eigenenergies');
75      xlabel('Eigenvalue number');
76      ylabel('Energy (eV)');
77
78      % Plot eigenenergies as points
79      for i = 1:numEigenvaluesToPlot
80          plot(i, energies_eV(i), 'bo', 'MarkerFaceColor', 'b');
81      end
82      hold off;
83
84      % Display calculated and theoretical energies
85      if V_type == 1 || V_type == 3 || V_type == 2
86          disp('Quantum Well Specifications:');
87          fprintf('Well Type: %s\n', getWellType(V_type));
88          fprintf('Width of the Well (nm): %.2f\n', L_nm);
89          if V_type == 2 % Finite Square Well
90              fprintf('Height of the Well (eV): %.2f\n', V0_eV);
91          elseif V_type == 3 % Harmonic Oscillator
92              fprintf('Spring Constant (eV/nm^2): %.2f\n', k_eV_per_nm2);
93          end
94          fprintf('Effective Mass (ratio to electron mass): %.2f\n', m_eff);
95          fprintf('Number of Grid Points: %d\n', N);
96
97          disp('Calculated and Theoretical Energies (eV):');
98          for i = 1:numEigenvaluesToPlot
99              fprintf('n = %d: Calculated = %.4f eV, Theoretical = %.4f eV\n', ...
100                         i, energies_eV(i), theoreticalEnergies(i));
101         end
102     end
103
104     % Helper function to get the well type as a string
105     function wellType = getWellType(typeNum)
106         switch typeNum
107             case 1
108                 wellType = 'Infinite Square Well';
109             case 2
110                 wellType = 'Finite Square Well';
111             case 3
112                 wellType = 'Harmonic Oscillator';
113             otherwise
114                 wellType = 'Unknown';
115         end
116     end
117
118
119     % Plot the potential V(x) and eigenfunctions psi(x)
120     figure;
121     hold on;
122     title('Potential and Eigenfunctions');
123     xlabel('Position (nm)');
124     ylabel('Energy (eV)');
125
126     % max_energy = max(energies_eV(1:numEigenvaluesToPlot));
127
128     % Plot the potential for the harmonic oscillator
129     if V_type == 3
```

```matlab
130          psi = abs(psi);
131          plot(x * 1e9, V / e, 'k-', 'LineWidth', 2, 'DisplayName', 'Potential');
132      end
133
134      % Plot eigenfunctions offset by their eigenenergies
135      for i = 1:numEigenvaluesToPlot
136          % Offset each eigenfunction by its eigenenergy
137          offset = energies_eV(i);
138          plot(x * 1e9, psi(:,i) + offset, 'DisplayName', ['Eigenfunction ' num2str(i)]);
139      end
140
141      legend show;
142      hold off;
143 end
```

Listing 1: Schrodinger Solver MATLAB Code

B Analytical Solution for Infinite well

Suppose we have a system where a (non-relativistic) particle is trapped in a one-dimensional well of length L. Inside the well there is no potential energy, and the particle is trapped inside the well by "walls" of infinite potential energy. Therefore, we have

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \tag{23}$$

Solving the Schrödinger equation for the region where the potential, $V(x)$, is ∞, we have:

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

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

$$(\infty)\psi(x) = E\psi(x)$$

This yields the solutions, $E = \infty$ and $\psi = 0$. $E = \infty$ is physically impossible (no particle has infinite energy) so we discard it.

For, $\psi = 0$, the particle can never be found outside of the well, only inside, according to the formulation of the question. Therefore, for the region $0 < x < L$ we have:

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

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

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

The general solution for the above differential equation is:

$$\psi(x) = A\sin(kx) + B\cos(kx) \; ; \; k = \sqrt{\frac{2mE}{\hbar^2}}$$

$\psi(x)$ and $\psi'(x)$ must be continuous at the boundaries $x = 0$ and $x = L$. For $x = 0$ we have:

$$\psi(x = 0^-) = \psi(x = 0^+)$$

$$0 = A\sin(0) + B\cos(0)$$

therefore, $B = 0$.

For $x = L$ we have:

$$\psi(x = L^-) = \psi(x = L^+)$$

$$0 = A\sin(kL)$$

$$kL = n\pi$$

$$k = \frac{n\pi}{L}$$

which gives:

$$\psi(x) = A\sin(\frac{n\pi x}{L})$$

A can be found by the normalization condition

$$\int_{-L}^{L} \psi^2 \, dx = 1$$

$$A^2 \int_{-L}^{L} sin^2(\frac{n\pi x}{L}) \, dx = 1$$

$$A = \frac{1}{\sqrt{L}}$$

Therefore, the wavefunction can be constructed as follows:

$$\psi(x) = \frac{1}{\sqrt{L}} sin(\frac{n\pi x}{L})$$

and the allowed energies can be constructed as:

$$\frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{n^2\pi^2}{L^2} = \frac{2mE}{\hbar^2} \quad ; \hbar = \frac{h}{2\pi}$$

$$E = \frac{h^2 n^2}{8mL^2}$$

$$E = n^2 \frac{h^2}{8mL^2} \quad \text{for} n = 1, 2, 3...$$

$$E_1 = \frac{h^2}{8mL^2}$$

Therefore, we have:

$$E_n = n^2 E_1$$

Now substituting $L = 4 \times 10^{-9}$ and $E_1 = .2 \, eV$, we get:

$$E_2 = 2^2 \times .2 = .8 \, eV \quad ; E_3 = 3^2 \times .2 = 1.8 \, eV \quad ; E_4 = 4^2 \times .2 = 3.2 \, eV$$

and

$$\psi_n(x) = \frac{1}{\sqrt{4 \times 10^{-9}}} sin(\frac{n\pi x}{4 \times 10^{-9}}) \quad \text{for} n = 1, 2, 3...$$