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Numerical Solution of Square Well Potential With Matrix Method Using Worksheets

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Abstract

We solve the time-independent Schrödinger equation for a square well potential, using matrix methods based numerical technique. Implementation of numerical method in a computer requires limiting the region of potential from infinity to some finite value, which is equivalent to embedding it within an infinite well potential. The eigen functions of the infinite well are utilised as the basis to build the hamiltonian matrix for the system. The matrix eigen equation is solved using Free Open Source Software (FOSS) Gnumeric which is a worksheet based environment that is easy for Implementation at the UG level.

1 Introduction

Marsiglio et.al., have introduced matrix methods for solving various quantum mechanical potentials [1, 2, 3] by embedding them within an infinite potential. This technique has the advantage of obtaining the energy eigen values and the corresponding eigen functions in a single iteration. With many FOSS offering eigen value solvers, this technique is easy to implement as part of simulation activities for quantum mechanics lab course at the UG level. Simulations have become an important approach for learning the concepts of physics[4, 5, 6]. There are many good simulations available at PhET [7, 8] and Compadre websites [9] written in Java and available for running both online and offline in order to understand the effect of various system parameters and their inter-relationships. Understanding and implementing the numerical methods involved to simulate a physical system is an important skill that needs to be developed while training to be a good physicist. Here, we focus on the pedagogical aspects involved in learning to perform simulations at the UG level, by taking the example of square well potential, which students encounter in introductory course of quan-

tum mechanics.

2 Methodology

To solve any physics problem using a computer simulation, we take up the following approach:

Step 1: Modelling the Physics problem

The primary step is to have clear understanding of ***Mathematical model*** that describes the problem at hand. Here, one could use the modeling methodology suggested by Hestenes [10] to ***describe*** the system w.r.t. its interactions and process involved in it. After giving full description of the system, one can proceed to ***formulate*** the model by introducing the force or potential obtained from the ***interaction law*** into the ***dynamical law*** that underlies the process and introducing the appropriate ***initial*** and ***boundary conditions*** that need to be complied with. Once, the mathematical model is ready, one can solve the problem using analytical technique, if available or alternatively one can resort to numerical methods.

Step 2: Preparing the system to be solved using numerical approach

- **Choice of Numerical Technique**
  By looking at all the available numerical methods for solving the current problem, one has to arrive at the technique that is ***stable***, ***accurate*** and ***reasonably fast*** among the various methods available.

- **Rephrasing the Physics problem in appropriate units**
  This is important so as to avoid very large or very small numbers in computation that could lead to round off errors. Here, either the variables involved are made dimensionless or have to be expressed in an appropriate set of units. For example, for astronomical systems, one can use astronomical units such as specifying the masses in terms of mass of earth and distances in terms of distance between Sun and Earth, time in light years and so on.

- **Discretizing the continuous variables**
  As the computer can handle only discrete data, it is inevitable to sample the continuous variable with appropriate step size and also limit the variables to a finite range in accordance with the region of interest for solving the problem. This is a must to translate the problem into one that could be programmable.

Step 3: Implementation of the numerical method in computer

- **Algorithm**
  The inputs required, the equations to be iterated, the functions that need to be called in the main processing block and outputs generated (to be displayed as tabular data or plots) needs to be clearly defined in a step by step procedure so

that it is easy to program in a chosen software. Then, the code is written.

- **Running the program**
  This is initially to be taken up for a problem for which we know the analytical solution. This helps to troubleshoot the code for any mistakes and ensures its proper working.

- **Varying the parameters related to the numerical algorithm**
  We have to run the code by changing the various inputs parameters that effect the algorithm to minimize the various errors associated with them. Typical parameters that need to be optimized would be step-size, number of points representing the variable, tolerance limits on the iterated-quantities, values that need to remain constant with increasing number of iterations, etc.

Step 4: Simulation

- **Varying the physical properties associated with the physical system**
  Once the code is optimized, the variables associated with the physics of the problem can be varied. Plots & tabular data could be generated for understanding the relationships that would lead to analysis, interpretation & discussion of the results.

- **Modifications to the Physical system at hand**
  It is possible to vary the physics problem, in the sense, that the functions, initial conditions, boundary conditions, etc., involved are changed but yet the same numerical technique could be employed to study the system.

3 Implementation

3.1 Modelling the Physics Problem:

Consider a microscopic particle in 1-Dimensional system (***reference system***)such as an electron which is of mass m and energy E (***object variables***) is interacting with a finite attractive potential well of width 'b' and depth V_0 (***interaction variables***). The interaction potential V(x) can be written in equation form as

$$V(x) = \begin{cases} V_0, & -\infty < x < -b/2 \\ 0, & -b/2 \leqslant x \leqslant b/2 \\ V_0, & b/2 < x < \infty \end{cases} \qquad (1)$$

and is plotted below in Figure 1.

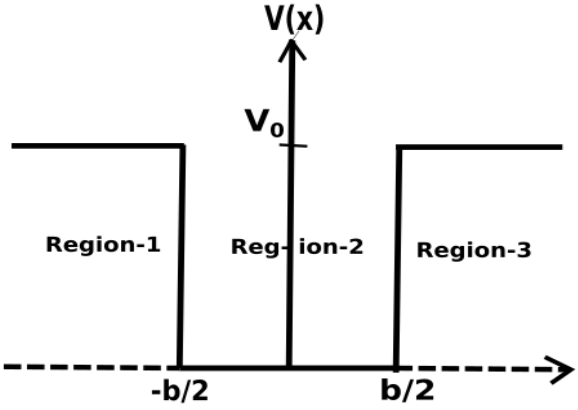

Figure 1: Finite square well in 1-D

In the microscopic domain, considering that the wave nature associated with a particle plays significant role in understanding the probability of it being found at various locations (dependent on ***state function***, ψ(x)), we need to solve the 'Time Independent Schrödinger Equation(TISE)' (***dynamical equation***) in the regions 1, 2 and 3, to obtain the wave functions for the particle with energy E i.e

$$H\psi(x) = E\psi(x) \tag{2}$$

where H is the hamiltonian of the system given by

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

Considering the case $E < V_0$, the analytical bound state solutions of TISE involving graphical approach have been discussed in various standard texts of quantum mechanics[11, 12, 13].
Taking specific values for parameters V_0 and b as: $V_0 = 14eV$ and $b = 2\mathring{A}$, we obtained the energy values for bound states by solving the eigen value conditions [11], utilising ***Newton-Raphson method***[14, 15] to 3 decimal places as

$$\begin{aligned} E1 &= 1.467eV \\ E2 &= 5.711eV \\ E3 &= 11.918eV \end{aligned} \tag{4}$$

Now, we focus on getting numerical solutions by using matrix diagonalization method suggested by Marsiglio [3, 16].

3.1.1 Marsiglio's matrix method

The central idea in matrix matching method is to limit the potential of interest to a finite region, which is equivalent to embedding it within an infinite square well potential of width 'a'. The TISE eq.(2) gets modified as

$$\Big[H_\infty + V_w(x)\Big]\psi(x) = E\psi(x) \tag{5}$$

where H_∞ is the hamiltonian of infinite square well potential and $V_w(x)$ is the potential limited to finite region [0,a].
The energy eigen values and normalized eigen functions of H_∞ are given by

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

and

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

This suggests the solution $\psi(x)$ to be written as a linear combination of sine functions as basis. So, $\psi(x)$ is expressed as

$$\psi(x) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} C_n sin\left(\frac{n\pi x}{a}\right) \tag{8}$$

where the coefficients C_n's need to be determined. This is akin to performing Fourier analysis.
Substituting eq.(8) in eq.(2), we get

$$H\sum_{n=1}^{\infty} C_n\Phi_n(x) = E\sum_{n=1}^{\infty} C_n\Phi_n(x) \tag{9}$$

Pre multiplying eq.(9) by $\Phi_m^*(x)$ on both sides and integrating over all space,

$$\int_{-\infty}^{\infty}\left(\Phi_m^*(x)\left[H_\infty + V_w(x)\right]\sum_{n=1}^{\infty}C_n\Phi_n(x)\right)dx = E\int_{-\infty}^{\infty}\left(\Phi_m^*(x)\sum_{n=1}^{\infty}C_n\Phi_n(x)\right)dx \tag{10}$$

Since integration and hamiltonian are linear operators, eq.(10) can be written as

$$\sum_{n=1}^{\infty}C_n\int_{-\infty}^{\infty}\Phi_m^*(x)H_\infty\Phi_n(x)dx + \sum_{n=1}^{\infty}C_n\int_{-\infty}^{\infty}\Phi_m^*(x)V_w(x)\Phi_n(x) = E\sum_{n=1}^{\infty}C_n\int_{-\infty}^{\infty}\Phi_m^*(x)\Phi_n(x) \tag{11}$$

Introducing the notation for

$$\int_{\infty}^{\infty}\Phi_m^*(x)V_w(x)\Phi_n(x) = V_{mn} \tag{12}$$

using

$$H_\infty\Phi_n(x) = E_n^\infty\Phi_n(x) \tag{13}$$

and

$$\int_{-\infty}^{\infty}\Phi_m^*(x)\Phi_n(x) = \delta_{mn} \tag{14}$$

we get

$$E_m^\infty C_m + \sum_{n=1}^{\infty}V_{mn}C_n = EC_m \tag{15}$$

for m=1, 2, 3,...

These are any array of m equations that can be expressed as

$$E_m^\infty C_{m\times1} + V_{m\times n}C_{n\times1} = EC_{m\times1} \tag{16}$$

Because m takes same values as n, we have

$$HC = EC \tag{17}$$

where

$$H = \begin{bmatrix} E_1^\infty + V_{11} & V_{12} & . & . & . & V_{1n} \\ V_{21} & E_2^\infty + V_{22} & . & . & . & V_{2n} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ V_{n1} & V_{n2} & . & . & . & E_n^\infty + V_{nn} \end{bmatrix}$$

and

$$C = \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ . \\ . \\ . \\ C_n \end{bmatrix}$$

or we can express H as

$$H_{n\times n} = E_n^\infty I_{n\times n} + V_{n\times n} \tag{18}$$

3.2 Application to finite square well potential

The hamiltonian for the finite square well potential is given by

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = H_\infty + V_w(x) \tag{19}$$

where, H_∞ is the hamiltonian of infinite square well potential and $V_w(x)$ is restricted to a finite region [0,a] defined as

$$V_w(x) = \begin{cases} V_0, & \text{if } b1 \leqslant x \leqslant b2. \\ 0, & \text{if } 0 < x < b1 \text{ and } b2 < x < a \\ \infty, & \text{x=0 and x=a} \end{cases} \tag{20}$$

and is shown in Figure 2.

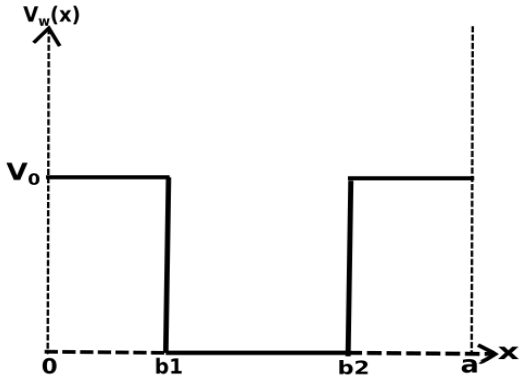

Figure 2: Square well embedded inside an infinite well

Now, V-matrix consists of diagonal elements, V_{nn} for which m=n and can be determined as

$$V_{nn} = \frac{n^2\pi^2}{2a^2} + \frac{V_0}{a}\Bigg[b1 + a - b2 + \frac{a}{2n\pi}(sin(\frac{2n\pi b2}{a}) - sin(\frac{2n\pi b1}{a}))\Bigg] \quad (21)$$

and non-diagonal elements, V_{nm} which are to be determined as

$$V_{nm} = V_0\Bigg[\frac{sin\frac{(n-m)\pi b1}{a}}{(n-m)\pi} - \frac{sin\frac{(n-m)\pi b2}{a}}{(n-m)\pi} + \frac{sin\frac{(n+m)\pi b2}{a}}{(n+m)\pi} - \frac{sin\frac{(n+m)\pi b1}{a}}{(n+m)\pi}\Bigg] \quad (22)$$

Theoretically, H-matrix is infinite in dimensions, which needs to be limited to a finite dimension, say N for sake of computation.

3.3 Choice of units: Atomic units

We prefer to work with atomic units where $\hbar$, m_e, c and Coulomb factor, $k_e = \frac{1}{4\pi\epsilon_0}$ all are equal to unity. This would mean that distances are choosen in Bohr and energies are in hartree[17]. That is,

$$L = 1Bohr = 0.52917725\mathring{A}$$
$$E = 1\ hartree = 27.211396\ eV$$

3.4 Discretizing position variable

We can only represent the position variable at certain discrete points within the finite region[0,a]. Typically, it is chosen as equally spaced points over this region with step size of say, h. That is, the values of x are limited to [0,h,2h,3h,....nh,...a].

3.5 Implementation in Gnumeric Spreadsheet

We enlist the various steps involved in implementing matrix method formalism for obtaining the energy spectrum and wave functions of 1-dimensional square well problem using free open source software, **'Gnumeric'** which is a spreadsheet environment.

Step 1 : **Initializing the parameters**

	A	B	C
1	**I-D Square well potential**		
2	**Initializing the parameters**		
3			
4	$V_0(x)$=	14.000	0.514
5	a=	8.000	15.118
6	b=	4.000	7.559
7	b1=	(a-b)/2	3.779
8	b2=	(a+b)/2	11.338

Figure 3: Initializing the various input parameters in gnumeric worksheet

The initial values to the various parameters, $V_0 = 14eV$, $a = 8\mathring{A}$ and $b = 4\mathring{A}$ involved in square well potential are entered in worksheet (as shown in Figure 3):

• In cells A4, A5, A6, we mention the parameters as labels.

• In cells B4, B5, B6 we enter their respective values as 14, 8 and 4.

• In cell C4, we have given formula $'' = \$B\$4/27.211396''$ so as to convert the potential $V_0(x)$ into hartree units and in cells C5 and C6 we have given the formula $'' = \$B\$5/0.52917725''$ and $'' = \$B\$6/0.52917725''$ respectively so as to convert the distances ('a' and 'b') into Bohr units.

• In cells A7 and A8 we label the parameters b1 and b2 respectively and show their respective formulae in B7 and B8. In cells C7 and C8, we enter the formulae as $'' = (\$C\$5 - \$C\$6)/2''$ and $'' = (\$C\$5 + \$C\$6)/2''$, respectively.

Step 2: Generating the hamiltonian matrix

Initially, let's choose 5 basis functions, N = 5, so we need to generate a 5×5 matrix. Now, we give the values of m & n from 1 to 5 in cells A17-A21(rows) and B16-F16(columns) as shown in Figure 4. Next, enter the formula for H-matrix in cell B17 as shown using **if condition expression** which is $'' = if(condition, [truevalue], [falsevalue])''$

In our case, the if condition is given as: $\$A17 = B\$16$. True value is for diagonal elements given by eq. (21), which is to be typed as

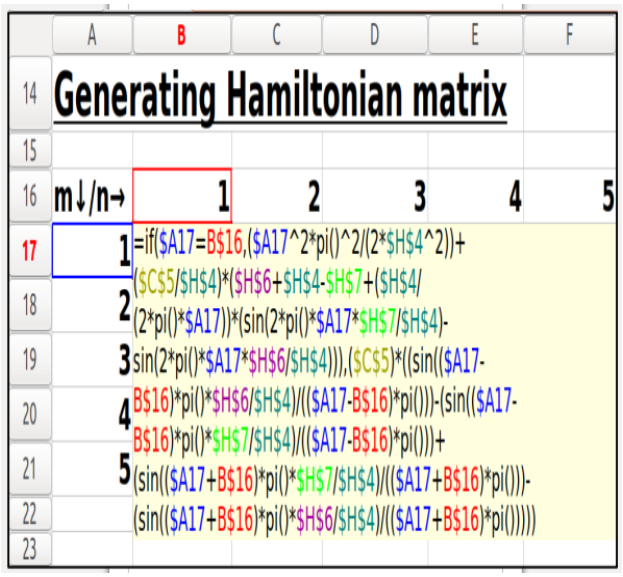

Figure 4: Generating the matrix in gnumeric sheet

```
($A17^2*pi()^2/(2*$C$5^2))+
($C$4/$C$5)*($C$7+$C$5-$C$8+
($C$5/(2*pi()*$A17))*
(sin(2*pi()*$A17*$C$8/$C$5)-
sin(2*pi()*$A17*$C$7/$C$5)))
```

whereas false value is for non-diagonal elements, given by eq.(22), and is typed as:

```
($C$4)*((sin(($A17-B$16)*pi()*
$C$7/$C$5)/(($A17-B$16)*pi()))-
(sin(($A17-B$16)*pi()*$C$8/$C$5)/
(($A17-B$16)*pi()))+(sin(($A17+B$16)*
pi()*$C$8/$C$5)/(($A17+B$16)*pi()))-
(sin(($A17+B$16)*pi()*$C$7/$C$5)/
(($A17+B$16)*pi())))
```

After entering desired formula, press Enter key, first matrix element will appear in cell

B17. To generate remaining values select cell B17 and drag the cursor upto cell F17 horizontally. After this, select entire row from B17:F17 and drag the cursor vertically and drop at F21. The complete H matrix having 25 elements is shown in Figure 5. **Step** hartree, we need to convert them into original units i.e in eV by multiplying with a factor of 27.211396 so as to compare with analytical values and this is done by typing formula in cell B35 as: " $= B\$28 * 27.211396$" and drag cursor upto F35.

	A	B	C	D	E	F
13	**Hamiltonian matrix elements**					
14						
15	**m↓/n→**	**1**	**2**	**3**	**4**	**5**
16	**1**	0.115	0.000	0.164	0.000	0.055
17	**2**	0.000	0.344	0.000	0.218	0.000
18	**3**	0.164	0.000	0.506	0.000	0.164
19	**4**	0.000	0.218	0.000	0.603	0.000
20	**5**	0.055	0.000	0.164	0.000	0.764

Figure 5: 5×5 H matrix in gnumeric sheet

	A	B	C	D	E	F
25	**Eigen values and eigen vectors**					
26						
27	**Ei→**	**E5**	**E4**	**E3**	**E2**	**E1**
28	**E(hartree)**	**0.864**	**0.727**	**0.466**	**0.219**	**0.056**
29	**Ci1**	0.166	0.000	0.301	0.000	0.939
30	**Ci2**	0.000	0.495	0.000	0.869	0.000
31	**Ci3**	0.472	0.000	0.812	0.000	−0.344
32	**Ci4**	0.000	0.869	0.000	−0.495	0.000
33	**Ci5**	0.866	0.000	−0.501	0.000	0.007
34						
35	**E(eV)**	**23.513**	**19.784**	**12.678**	**5.967**	**1.511**

Figure 6: Calculating eigen values and eigen functions

3: **Calculating the eigenvalues and corresponding eigenvectors**

Gnumeric has an eigen value solver, which is not available in other worksheet environments such as MS-excel or open Office Calc. Here, we have generated 5×5 matrix in Step 2 which has 5 eigen values and 5×1 eigen vector for each of them. Now, select 6×5 matrix from B28 to F33 by dragging the mouse and then we type in formula bar:
" $= eigen(B17 : F21)$"
and press Ctrl+Shift+Enter keys together. With this, all 5 eigen values will appear in cells B28:F28 in decreasing order along with their corresponding 5 column vectors below each of them as shown in Figure 6.
Since all energy values come out to be in

Step 4: **Generating basis functions**

In order to determine the wavefunctions in eq.(8), we need to generate the basis functions, $\phi_n(x)$. In Figure 7, we generate x-values first from A43:A58 at an interval of 1 i.e 16 values and the values of 'n' are to be fed in cells B41:F41 as 1, 2, 3, 4, 5. The cells B42:F42 are labelled for clarity as $phi_1(x)$, $phi_2(x)$, $phi_3(x)$, $phi_4(x)$ and $phi_5(x)$ respectively. Now, select the entire array i.e. range of cells from \$B43:\$B58 and then enter in formula bar:

```
=sqrt(2/$C$5)$sin(B$41*pi()*
($A43:$A58)/$C$5)
```

	A	B	C	D	E	F
39	**Generating basis function(phi(x))**					
40						
41	x↓/n→	1	2	3	4	5
42		$phi_1(x)$	$phi_2(x)$	$phi_3(x)$	$phi_4(x)$	$phi_5(x)$
43	0	=sqrt(2/$C$5)*sin(B$41*pi()*($A43:$A58)/$C$5)				
44	1	0.075	0.147	0.212	0.269	0.313
45	2	0.147	0.269	0.345	0.362	0.318
46	3	0.212	0.345	0.348	0.220	0.009
47	4	0.269	0.362	0.220	−0.066	−0.309
48	5	0.313	0.318	0.009	−0.309	−0.322
49	6	0.345	0.220	−0.205	−0.350	−0.018
50	7	0.361	0.084	−0.342	−0.163	0.304
51	8	0.362	−0.066	−0.350	0.130	0.326
52	9	0.348	−0.205	−0.227	0.339	0.027
53	10	0.318	−0.309	−0.018	0.326	−0.299
54	11	0.275	−0.360	0.198	0.101	−0.330
55	12	0.220	−0.350	0.339	−0.190	−0.036
56	13	0.155	−0.280	0.352	−0.357	0.294
57	14	0.084	−0.163	0.233	−0.291	0.334
58	15	0.009	−0.018	0.027	−0.036	0.044

Figure 7: The five basis functions of infinite square well potential

After giving the formula, press Ctrl+Enter. The remaining phi vectors will be generated by cursor drag from $B43:$B58 and drop at $F43:$F58. We can observe that all these phi functions are nothing but the 5 sine functions of 1-D infinite square well.

Step 5: **Obtaining the wave functions**

For obtaining the wave functions, x values are generated first ranging from 0-15 in cells A64:A79 just as we have done in Step 4. Now, we need to multiply eigen vectors with basis functions to get wave functions(psi) as per eq. (7) By looking into Figure 6 and Figure 7 one can generate fifth wavefunction as

$psi_5(x) = C51 * phi_1(x) + C52 * phi_2(x) + C53 * phi_3(x) + C54 * phi_4(x) + C55 * phi_5(x)$

where C51, C52, C53, C54, C55 are the components of 5th eigen vector(coefficients of fifth wave function) from B29:B33. To determine this, first select the range of cells from B64:B79 and then enter the following expression in the formula bar as:

$= \$B\$29 * \$B43 + \$B\$30 * \$C43 + \$B\$31 * \$D43 + \$B\$32 * \$E43 + \$B\$33 * \$F43$

and press Ctrl+Enter. This will generate only fifth wavefunction. In order to generate all ψ functions, one needs to give the formula in such a way that all ψ values will appear simultaneously. To achieve this, first select the range of cells from B64:F79 and then enter the following in the formula bar.

$= B\$29 * \$B43 + B\$30 * \$C43 + B\$31 * \$D43 + B\$32 * \$E43 + B\$33 * \$F43$

and press Ctrl+Enter, which will generate all the ψ values as shown in Figure 8. It is to be observed that ψ functions that are generated are in descending order.

	A	B	C	D	E	F
61	**Wave functions**					
63	x↓/psi(x)→	$psi_5(x)$	$psi_4(x)$	$psi_3(x)$	$psi_2(x)$	$psi_1(x)$
64	0	0.000	0.000	0.000	0.000	0.000
65	1	0.384	0.306	0.038	−0.005	0.000
66	2	0.462	0.448	0.165	0.054	0.022
67	3	0.207	0.361	0.342	0.191	0.080
68	4	−0.119	0.122	0.414	0.348	0.175
69	5	−0.223	−0.111	0.263	0.429	0.289
70	6	−0.055	−0.196	−0.054	0.364	0.394
71	7	0.162	−0.100	−0.321	0.153	0.459
72	8	0.177	0.081	−0.338	−0.122	0.463
73	9	−0.026	0.193	−0.093	−0.346	0.404
74	10	−0.215	0.131	0.231	−0.430	0.303
75	11	−0.147	−0.090	0.408	−0.363	0.188
76	12	0.166	−0.338	0.359	−0.210	0.089
77	13	0.447	−0.449	0.186	−0.067	0.026
78	14	0.413	−0.334	0.048	0.003	0.001
79	15	0.053	−0.040	0.002	0.002	0.000

Figure 8: The wave functions of square well potential

4 Results and Discussions

4.1 Visualising wavefunctions and probability densities

Plotting the wave functions '$\psi_n(x)$':
We plot the first three wavefunctions as a superposition of the basis functions with their corresponding weightages (coefficients). The plots are shown in Figure 9.

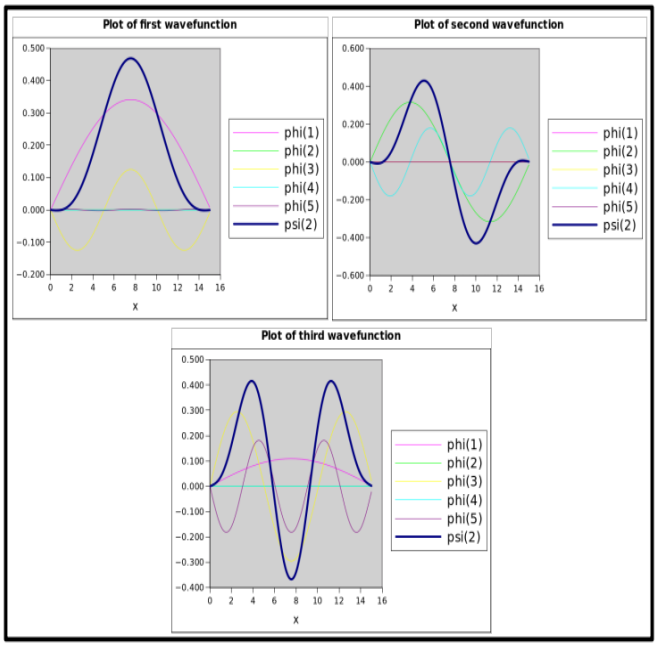

Figure 9: Graph of $\psi_1(x)$, $\psi_2(x)$ and $\psi_3(x)$ eigen functions

Probability density functions :
Once we obtain the wavefunctions, we can determine probability densities i.e probability of finding a particle(electron) in state $\psi(x)$ at position x by multiplying conjugate of ψ with ψ i.e $||\psi|| = \psi^*\psi$. The probability densities corresponding to first three wavefunctions which are of our interest are shown in Figure 10.

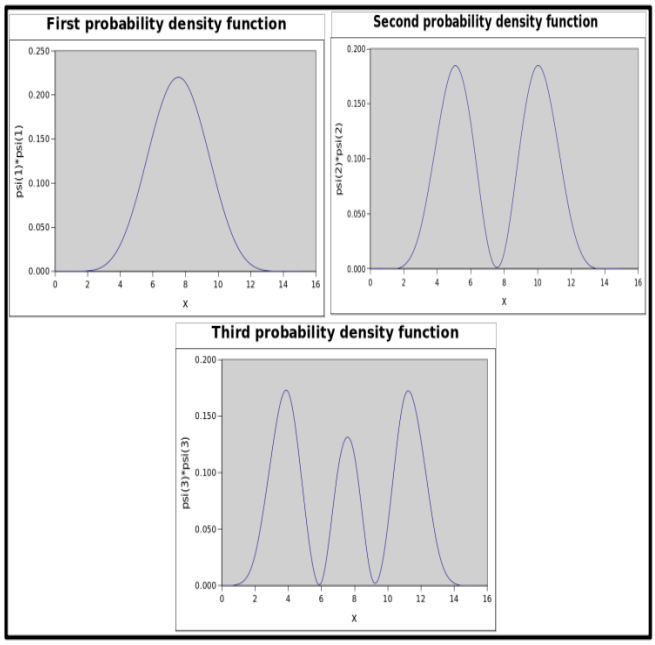

Figure 10: Getting the probability densities for square well potential

4.2 Study of variation of algorithm parameters: N and a

Effect of number of basis functions 'N':
During the implemetation stage, we have generated the results for N = 5 but these do not give the expected energy values to a good accuracy. So, we increased N in steps of 5 upto N=30, where the accuracy is found to be less than 2%. This effect could be clearly seen in Table 1.

Table 1: Comparison of numerical and analytical energy values for a particle in finite square well for $V_0 = 14eV = 0.514$ hartree and $a = 8\mathring{A}$=15.118 Bohr

	Energy eigen values(eV)			
	Analytical	Numerical		
		N=5	N=30	N⩾70
E1	1.467	1.511 (3.00%)	1.468 (0.07%)	1.468 (0.07%)
E2	5.712	5.967 (4.48%)	5.722 (0.19%)	5.721 (0.17%)
E3	11.919	12.678 (6.38%)	12.089 (1.43%)	12.087 (1.42%)

Effect of varying the infinite square well width 'a':
The effect of infinite square well of width(a) on bound state energy values is well presented in Table 2. It can be seen that the accuracy of given energy level decreases with the increase in 'a' for same value of N = 70. The explanation behind this is that as 'a' increases, spatial resolution gets decreased for particular basis state, ϕ_{30}(say) as compared to 30th basis state for smaller value of 'a'. Also, the spread of sine wave increases well beyond the region of interest. As a result, there will be poor representation of basis functions within the infinite square well region. Therefore, to achieve good convergence as 'a' is increased, we need to increase the number of basis functions, N and decrease the step-size, h for descretizing 'a' accordingly. Another important observation is that for well width b = $4A^o$, only for a $\geq$ 20 A^o, the numerical results converge to all the three analytical values.

4.3 Simulation by varying the physical parameters of the system: V_0 and b

Effect of varying the finite square well width 'b':
Results of bound state energies for finite square well potential as a function of well-width 'b' are shown in Table3. It is clear that as 'b' increases, number of bound states also increases.
As $b \to 0$, the finite square well reduces to a delta potential where the probability of finding a particle becomes maximum at the centre of infinite square well. On other hand, when $b \to a$, numerical results began to resemble with those of the infinite square well.
Effect of varying the finite square well depth $'V_0'$:

When infinite square well depth, V_0 is increased, the number of bound states also increased and such behaviour is also expected which can be seen clearly from data presented in Table 4. One can observe that the energy eigen values for $V_0 = 10^4$ are very close to those of the infinite well potential shown in last column.

Table 2: Variation of energy eigen values with infinite square well width 'a' for $b = 4\mathring{A} = 7.559$ Bohr and $V_0 = 14eV = 0.514$ hartree. N is varied till convergence is acheived.

	Energy eigen values(eV)						
	Analytical	Numerical					
		a=10Å		a=20Å		a=30Å	
		N=70	N=80	N=70	N=100	N=70	N=150
E1	1.467	1.467	1.467	1.467	1.467	1.468	1.467
E2	5.712	5.712	5.712	5.713	5.712	5.716	5.712
E3	11.919	11.954	11.954	11.921	11.919	11.926	11.919

5 Conclusions

We have introduced a simple worksheet based simulation methodology for solving the TISE for 1D finite square well for obtaining its bound state energy eigen values and corresponding eigen wavefunctions using the 1D infinite square well wavefunctions as basis. This approach could be easily extended to solve the Schrödinger equation for other potentials such as Harmonic, Anharmonic, Morse and Double well as well as N-square-well since it is possible to obtain the analytical expressions for the integrals involved in the determination of hamiltonian matrix elements for these. For central potentials such as Hydrogen atom, spherical square well, Yukawa and Woods-Saxon, we need to determine the integrals involved numerically and a FOSS Scilab is a good choice. Even then, the current suggested approach could be used as the first step to give clarity regarding the steps involved in implementation for the former potentials, so that it becomes pedagogically easy to write the code in Scilab for the later ones.

Table 3: Variation of energy eigen values with finite square well width(b) for $N = 140$, $a = 8\mathring{A} = 15.118$ Bohr and $V_0 = 14eV = 0.514$ hartree. The analytical value corresponding to energies are shown below in brackets.

	Numerical(Analytical) energy eigen values(eV)		
	b=2Å (a=20Å)	b=4Å (a=16Å)	b=6Å (a=16Å)
E1	3.915 (3.915)	1.467 (1.467)	0.756 (0.756)
E2	12.972 (12.972)	5.712 (5.712)	2.997 (2.997)
E3		11.919 (11.919)	6.619 (6.619)
E4			11.302 (11.302)

Table 4: Variation of energy eigen values with finite square well depth(V_0) for $N = 100$, $a = 20\mathring{A} = 15.118$ Bohr and $b = 4\mathring{A} = 7.559$ Bohr. The values written inside brackets are analytical results corresponding to energies.

	Numerical(Analytical) energy eigen values(eV)			
	Finite well			**Infinite well**
	V_0=50eV	V_0=1000eV	V_0=10^4eV	
E1	1.812 (1.812)	2.212 (2.212)	2.346 (2.346)	2.350
E2	7.214 (7.214)	8.846 (8.846)	9.383 (9.382)	9.401
E3	16.084 (16.084)	19.900 (19.900)	21.112 (21.110)	21.152
E4	28.135 (28.135)	35.373 (35.372)	37.533 (37.530)	37.603
E5	42.510 (42.510)	55.259 (55.258)	58.646 (58.640)	

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