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Harnessing the Matrix Method with SMath to Explore the Finite Square Well Potential

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Abstract. This innovative research makes use of a matrix-method driven numerical voyage into the foundation of the time-independent Schrödinger equation for a one-dimensional finite square well potential to unlock the secrets of the quantum realm. This is made possible by the unmatched power of the open-source computational juggernaut, SMath Studio. The work unfolds the quantum tapestry by cleverly placing the finite square well inside the infinitely large potential of an infinite square well, using an infinite number of basis vectors to invoke wavefunctions from the very fabric of the universe. This scholarly masterwork not only clarifies the elusive low-lying bound states of the finite square well potential but also acts as a quantum lighthouse, illuminating the complex quantum landscape for undergraduate students with unmatched clarity and understanding.

Keywords: SMath Studio, finite square well potential, infinite square well potential, matrix method

Introduction

Undergraduate physics enthusiasts embark on an intriguing quantum journey through the realm of quantum mechanics, which is dominated by the Schrödinger equation, which is the quantum analog of Newton's well-known second rule of motion. When they move through the introductory landscapes of quantum mechanics, they come across an area where the boundaries between the bound and the unbound are defined by the way that analytic solutions weave reality for a range of potentials. A unique window into the quantum world where energy and eigenfunctions are crystal clear is provided by the classic challenge of the one-dimensional infinite square well (ISW). The real intricacy of the quantum cosmos, however, is found elsewhere, in the finite potentials that control the enormous sphere spanning from nuclear secrets and atomic details to solid-state enigmas and the rapidly developing science of nanophysics. A new era of quantum exploration is being ushered in by the capacity to numerically solve the time-independent Schrödinger equation (TISE) for any potential, no matter how complex, thanks to the strength of current computing.

Within the sacred texts of basic quantum mechanics, the one-dimensional finite square well (FSW) potential stands as a pivotal chapter, sharing the stage with the legendary ISW (Griffiths, 2005). The journey through its mathematical landscape is nothing short of a heroic quest, as it conjures up transcendental equations that challenge the very boundaries of human intellect. Among the myriad of techniques to conquer these quantum enigmas, the graphical method has been an ancient ally, a beacon of clarity in the dense fog of complexity (Lima, 2020; Mallow, 1996; Knight, 2007; Guest, 1972; Garrett, 1979; Murphy & Phillips, 1976; Cameron Reed, 1990; Barker et al., 1991; Lindberg Vern, n.d.). Yet, as we delve deeper into the quantum abyss, a new savior emerges as the numerical solution of the TISE for any conceivable quantum potential (Marsiglio, 2009; Jelic & Marsiglio, 2012; Jugdutt & Marsiglio, 2013; Sastri et al., 2020). This noble technique, cradled within the vast expanse of the ISW

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potential, offers a bold alternative to the graphical odyssey, using eigenfunctions as the guiding stars in this celestial navigation. The hallowed grounds of the computing laboratory become a battleground for the minds of introductory quantum physics students. Here, amidst the digital forge, students are transformed into quantum warriors, their spirits enriched by the thrill of discovery. This active engagement is not merely academic; it is a rite of passage into the realm of quantum mastery, where understanding the fabric of the universe and wielding numerical techniques become the weapons of choice in the eternal quest for knowledge (Kinderman, 1990).

SMath Studio emerges as a distinguished Free Open-Source Software (FOSS), presenting itself as an eminent and cost-effective alternative to the more costly (Mathcad, thereby establishing its credentials as a formidable tool within the educational domain (Atkin, 2021). The notable work of Atkin, who adeptly resolved the TISE for the hydrogen atom using SMath Studio, serves as a testament to its capability, culminating in the creation of an instructional worksheet that stands as a beacon of academic utility. This scholarly endeavor significantly underscores the pedagogical implications, steering the academic discourse towards the adept application of numerical matrix diagonalization. This method, eloquently facilitated by SMath Studio, is lauded for its direct approach, offering a sophisticated yet accessible alternative to the conventional graphical or shooting methods traditionally employed for the derivation of energy eigenvalues and their corresponding eigenvectors. Such an approach not only enriches the educational experience but also broadens the methodological horizon for students and educators alike in the field of quantum mechanics.

Theoretical Background

The Hamiltonian of a particle confining in an infinite square well potential is defined as

$$H_\infty = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_\infty(x) \quad (1)$$

The first term on the right side of equation (1) is the kinetic energy operator and the second term is the potential energy operator. The matrix equation can be represented as

$$H_\infty\phi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + V_\infty\phi(x) \quad (2)$$

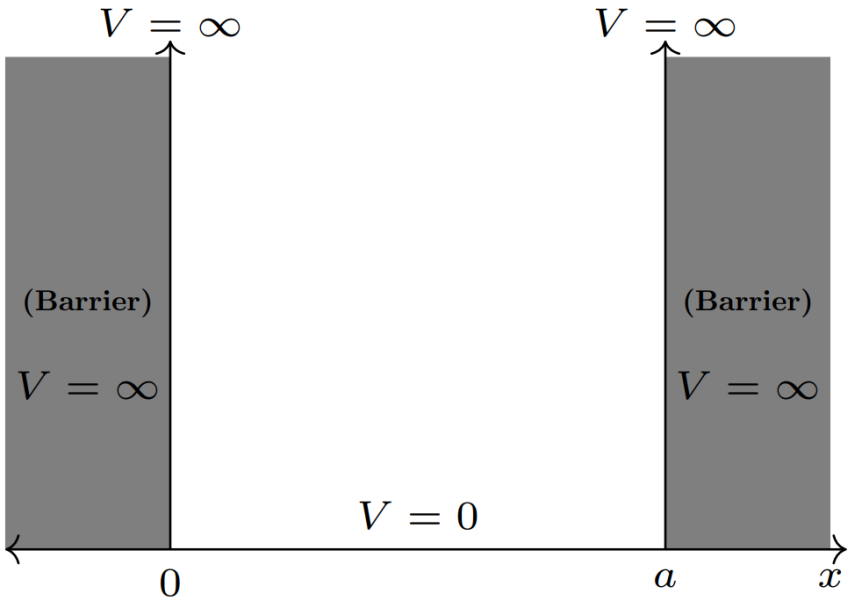


Figure 1. Finite square well potential embedded within an infinite square well potential

The potential energy of the infinite square well is

$$V_\infty(x) = \begin{cases} 0 & if\ 0 < x < a \\ \infty\ if\ x > a\ and\ x < 0 \end{cases} \quad (3)$$

On solving equation (1) imposing infinite potential term as in equation (3), the eigenfunctions and eigenvalues can be expressed as

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\right) & if\ 0 < x < a \\ \infty & otherwise \end{cases} \quad (4)$$

and

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = n^2 E_1 \qquad n = 1,2,3,\cdots \quad (5)$$

$E_1 = \pi^2\hbar^2/2ma^2$ is the ground-state energy of the particle.

The Hamiltonian for FSW potential embedded in ISW potential is defined as

$$H = H_\infty + V(x) \quad (6)$$

with a prototype potential of the form

$$V(x) = \begin{cases} V' & if\ c \le x \le d \\ 0 & if\ 0 < x < c\ \&\ d < x < a \\ \infty & otherwise \end{cases} \quad (7)$$

The Schrödinger equation is given by

$$H\psi(x) = E\psi(x) \quad (8)$$

When the particle in FSW potential is embedded in ISW potential, the eigenstate of the infinite square well potential can be treated as a basis to generate wave-function for FSW potential. Hence, ϕ_n in equation (4) is the basis, wave-function for FSW potential ψ can be represented as

$$\psi(x) = \sum_{q=1}^{\infty} C_q\, \phi_q(x) \quad (9)$$

where C_q are the eigenvector solving matrix equation of FSW potential. From equations.8 and 9 we can write

$$(H_\infty + V) \sum_{q=1}^{\infty} \phi_q\,(x) = E \sum_{q=1}^{\infty} C_n\, \phi_q(x) \quad (10)$$

Left multiplying by $\phi_q^*(x)$ to both sides of the equation 10 and integrating from 0 to a, the hamiltonian matrix element (Mallow, 1996) is found to be

$$H_{qp} = V'\left[\frac{\sin\left(\frac{(q-p)\pi d}{a}\right)}{(q-p)\pi} - \frac{\sin\left(\frac{(q-p)\pi c}{a}\right)}{(q-p)\pi} + \frac{\sin\left(\frac{(q+p)\pi c}{a}\right)}{(q+p)\pi} - \frac{\sin\left(\frac{(q+p)\pi d}{a}\right)}{(q+p)\pi}\right] \quad (11)$$

$$H_{qq} = \frac{n^2\pi^2}{2a^2} + \frac{V_0}{a}\left[a - b + \frac{a}{2q\pi}\left(\sin(2q\pi d/a) - \sin(2q\pi c/a)\right)\right] \quad (12)$$

where q and p indices represent rows and columns.

Choice of Units

In performing a computer solution of the Schrödinger equation, we need either to make dimensioned parameters dimensionless or use the appropriate units natural to the problems. As the physical problem underlying the microscopic level, we prefer to use atomic units where $\hbar = m = c = e = k_e = 1$. In this system, lengths are expressed in Bohr. $1\ bohr \equiv \frac{\hbar^2}{mk_e e^2} \approx 0.529\ ^\circ A$. The energies are expressed in Hartree.

$$1\ hartree\ \equiv \frac{mk_e^2 e^4}{\hbar^2} \approx 27.2114\ eV.$$

SMath Model of Finite Square Well Potential

Step-1: Parameter Initialization

The parameters related to our present problem of interest are supplied at the top of SMath worksheet. As the unit of parameter plays a crucial role, we have used parameters in the atomic

units. Considering an electron in a 20 ^{0}A-wide finite potential well of potential height $V' = 1.0$ eV, which are reasonable parameters for an electron in a semiconductor device (Knight, 2007). We set up the width of the infinite well with a=20 ^{0}A for the best result as discussed in Section 6. a_{max} and b_{max} represent a and b in the bohr unit.

Step-2: Hamiltonian Matrix Generation

In this study, we have followed the Marsiglio matrix method (Marsiglio, 2009). The diagonal matrix elements are determined by the function g. The first part of g is the kinetic energy of a particle in ISW potential and the second part indicates the potential energy terms that arise due to FSW potential. The potential function f creates off-diagonal matrix elements.

Here we have generated a 5×5 Hamiltonian matrix, the smallest possible matrix to find five energy eigenvalues including at least one unbound state, with the help of two *for*-loop with loop variables p and q run over the ranges 1 to 5. To compute the values of each matrix element, an *if-else* structure is used. ∨ symbol in $(p < q) \vee (p > q)$ shows boolean *OR* operation satisfying any conditions of $p < q$ and $p > q$. The TRUE condition generates the off-diagonal matrix elements whereas the FALSE condition generates diagonal matrix elements. Moreover, in our computation, we limit the computational values up to four decimal places so for a true condition we impose a case available in SMath which filters the matrix element values. It allows the values upto 10^{-4} otherwise, it rounds off to zero.

Step-3: Eigenvalues and Eigenvector Generation

The default SMath Studio as such has no functions to find eigenvalues and eigenvectors. Installation of 'DotNumerics' plugins facilitates to compute of eigenvalues and eigenvectors directly calling functions *dn_LinAlgEigenvalues()* and *dn_LinAlgEigenvectors()* respectively. The generated eigenvalues sometimes may not be sorted from lowest to highest value or reverse, so we have incorporated a little bit of extra code to avoid it. For this at first, we have stacked '*values*' and '*vector*' forming a matrix and then sorted the first row of the matrix in increasing values. When sorting occurs other row values do not sort and each column element lies below each eigenvalue. The matrix U is the required matrix whose first row is the eigenvalues and each column from the second row represents the eigenvector. All eigenvectors are stored as '*eigenvectors*' using '*eigenvectors: =remove Rows()*'.

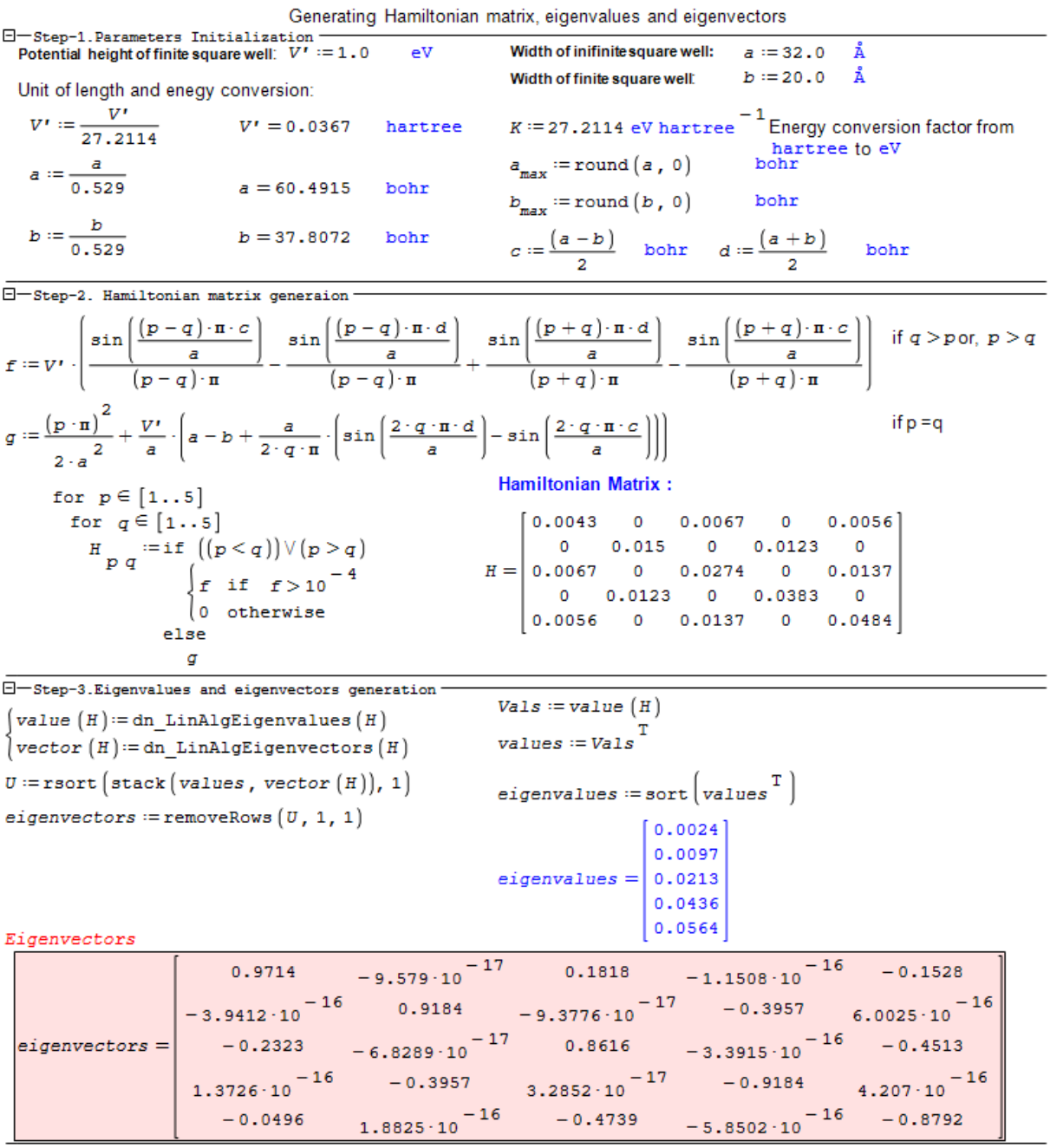


Figure 2. SMath worksheet for generating eigenvalues and eigenvectors from the Hamiltonian matrix

Step-4: Extracting Individual Eigenvalues and Eigenvectors

The individual eigenvalues and eigenvectors are extracted creating a *for* loop as shown at the top in Figure 3. The first line extract eigenvalues and the third line give corresponding eigenvectors. The second line converted the energy eigenvalues from the Hartree unit into eV. The v_1, v_2, v_3, v_4 and v_5 are eigenvectors corresponding to eigenvalues λ_1, λ_2, λ_3, λ_4 and λ_5 respectively.

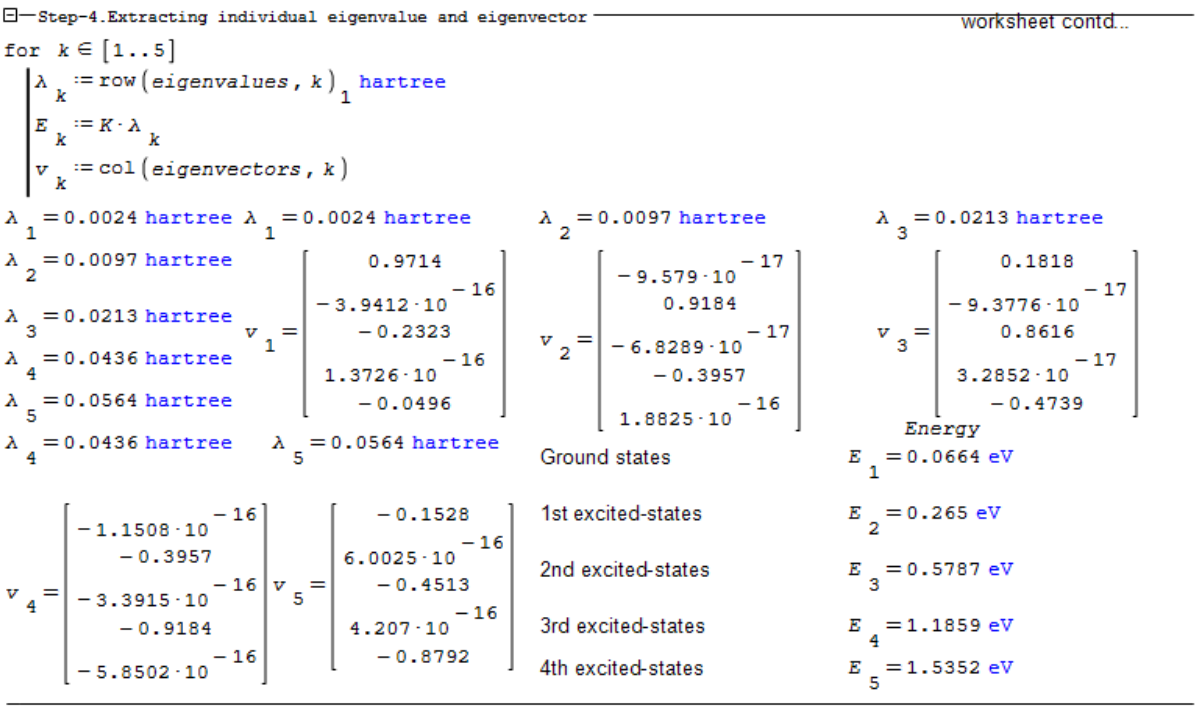


Figure 3. SMath Worksheet to extract individual eigenvalue, eigenvector

Step 5: Generating Basis Function

The basis function is generated using two nested *for*-loop using equation (Knight, 2007). The *for* loop controlled by the loop variable k changes from 1 to 5 and produces 5 columns whereas the x variable runs over the range 1 to a_{max} and generates 60 rows. The last line of the inner loop generates five basis functions Phi_1, Phi_2, Phi_3, Phi_4 and Phi_5 and the matrix element of each of them is stacked in 60 rows as 5 column matrix from left to right. eval function is used to speed up the computations.

Step-6: Generating Wave-function and Probability density functions:

In finding wave-functions $\Psi_n(x)$, each eigenvector components need to be multiplied with the corresponding basis function and add them. To compute each wave function a *for*-loop with controlling variable k running from 1 to 5 and the *sum (4)* option available in SMath is used.

$$psi_k = eval(\sum_{s=1}^{5}(v_k)_s \cdot Phi_s) \tag{13}$$

The components of each eigenvalue can be extracted from $(\text{v}_k)_s$ by setting k from 1 to 5 and s from 1 to 5. The probability density function is generated by forming a matrix using two nested *for* loops changing the loop variables k and i from (1 to 5) and (1 to 60) respectively. Each column of matrix p extracted using $P_k := col(p, k)$ gives each probability density (see Figure 4. For plotting wave functions against x, we have created a plotting matrix Psi using the *augment* function which combines the x values and computed psi values.

Wavefunction and probability worksheet contd...

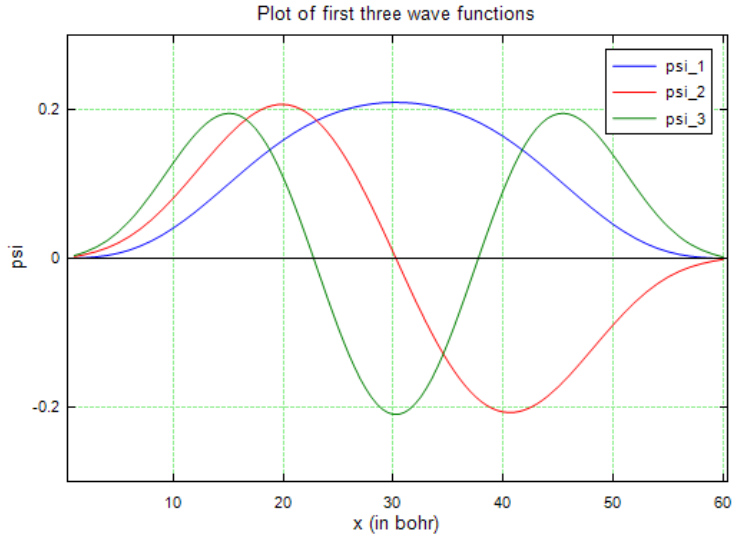
Step-5.Basis function

```
for n_x ∈ [1..5]
  for x ∈ [1..a_max]
    phi_{x,n_x} := eval(√(2/a) · sin((n_x · π · x)/a))
    Phi_{n_x} := col(phi, n_x)
```

Step-6.Generating Wave-functions and Probability density

```
x := [1..a_max]
for k ∈ [1..5]
  psi_k := eval(Σ_{s=1}^{5} (v_k)_s · Phi_s)
  for i ∈ [1..a_max]
    p_{i,k} := eval(psi_k)_i^2
    P_k := col(p, k)
  Psi_k := augment(x, psi_k)
  Prob_k := augment(x, P_k)
```

$$abs := \begin{bmatrix} 0 & 0 \\ a_{max} & 0 \end{bmatrix}$$



Psi_1
Psi_2
Psi_3
abs

Figure 4. Plots of wave functions

The positions are placed in the row x vector. Similarly, the *augment* function combines x and P_k values into the plotting matrix $Prob$ for probability density function plotting. The very versatile featured X-Y plot is used to plot wave functions and probability density functions. By left-clicking on the graph area, the formatting window appears. The required changes can be updated from there. The required matrix quantities (psi_1, psi_2 and psi_3) and ($Prob_1$, $Prob_2$ and $Prob_3$) to be plotted are inserted within the x-axis at psi=0 is drawn using matrix *abs*. As the X-Y plot in SMath Studio has no options to express mathematical symbols, subscripts and superscripts we have managed some symbolic expressions in easily understandable symbols. For example, we have expressed psi_1, psi_2 and psi_3 as *psi_1*, *psi_2* and *psi_3* respectively in X-Y plot.

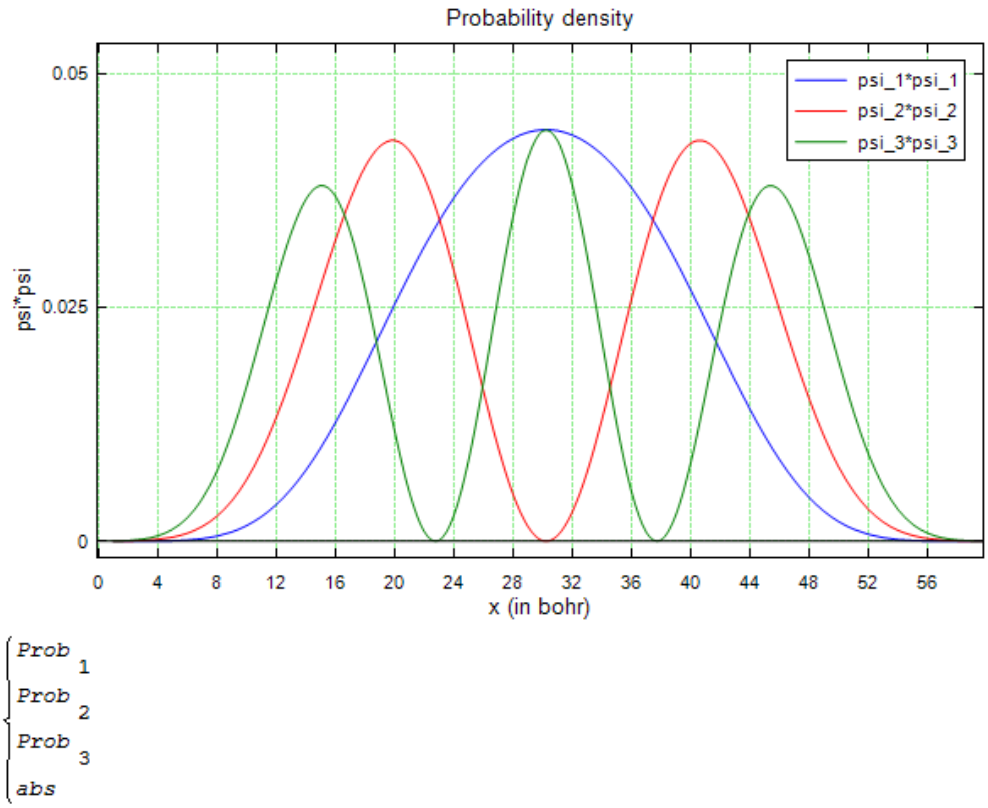
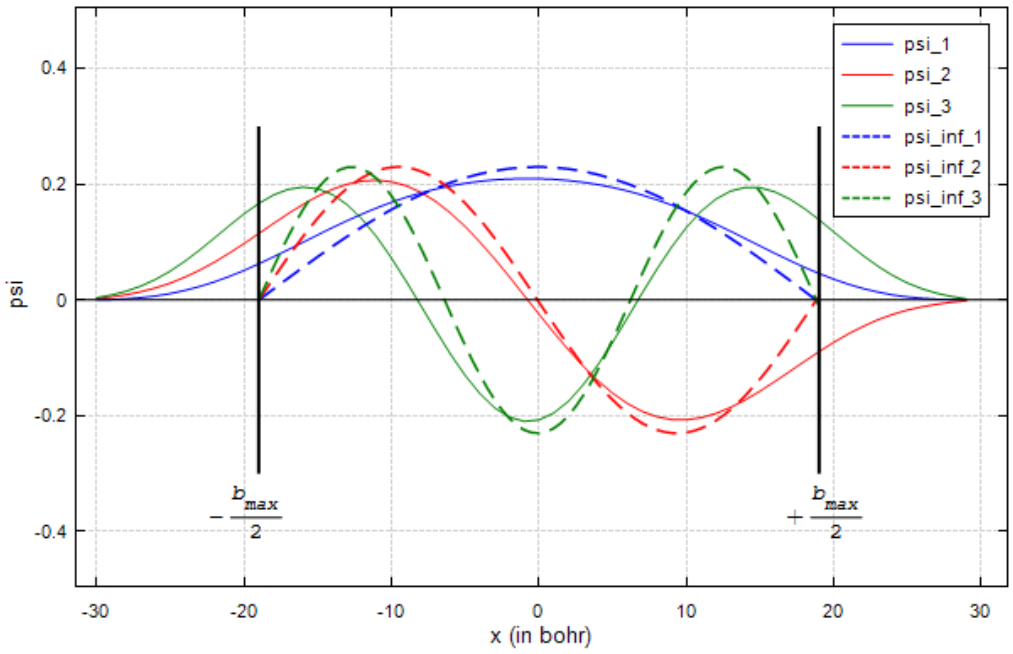


Figure 5. Plots of probability density functions

Results and Discussion

The first three wavefunctions are plotted in Figure 4. Figure 5 shows probability density functions against position x. As only the first three energy eigenvalues as shown in the second worksheet (See Figure 4) lie below $V' = 1.0\ eV$, formed bound states. The approximate energy values for the first four bound states found were listed in Table 1. If the wall positions of FSW and ISW as mentioned in equation (7) are replaced by the finite well walls at $(-b_{max}/2,\ +b_{max}/2)$ and $(-\mathrm{a}_{max}/2,+\mathrm{a}_{max}/2)$ respectively, the wavefunctions of FSW slowly convergence at $-\mathrm{a}_{max}/2$ and $+\mathrm{a}_{max}/2$ points whereas the wavefunctions of the ISW sharply converges at $-b_{max}/2$ and $+b_{max}/2$. The wavefunctions are shown in Figure 6. The wavefunctions for the ISW potential are drawn considering walls of infinite wells at positions $-\mathrm{a}_{max}/2$ and $+\mathrm{a}_{max}/2$ shrinks to $-b_{max}/2$ and $+b_{max}/2$ respectively. The matrices *left_side_well_position* and *right_side_well_position* is used to plot marker lines at $-b_{max}/2$ and $+b_{max}/2$ respectively. *psi_inf_1*, *psi_inf_2* and *psi_inf_3* represent the first three wavefunction for ISW potential.



Psi_1
Psi_2
Psi_3
Psi_inf_1
Psi_inf_2
Psi_inf_3
abs
left_side_well_position
right_side_well_position

Figure 6. Plots of wavefunctions of a particle in FSW and ISW potential with x wavefunctions for ISW potential is plotted assuming the walls at $-a_{max}/2$ and $+a_{max}/2$ shrinks to $-b_{max}/2$ and $+b_{max}/2$ respectively.

Variation of Energy with b/a

Finding energy values of the one-dimensional FSW potential embedded into an ISW potential depends on the b/a values. It is observed that the least energy eigenvalue which is best fitted with the exact energy of the ground state could be found at b/a close to 0.62. The variation of ground-state energy against b/a from 0 to 1.0 for $n = 5,30,80$ is plotted in Figure 7. The small variation of energy with b/a is depicted in the inset of Figure 7. It could be shown that one can get the least energy eigenvalue for any state at b/a$\sim$ 0.62.

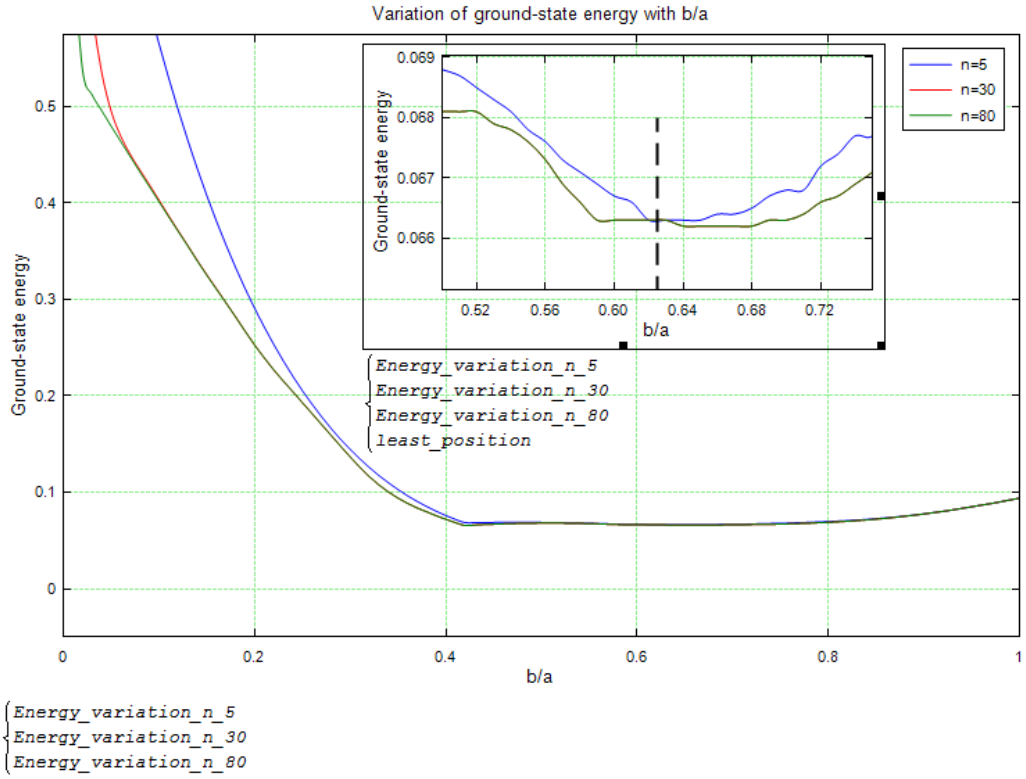


Figure 7. Plots of ground state energy of FSW potential with b/a

Table 1. Comparison of eigenvalues for finite potential width V ′ = 1.0 eV, a= 32 ˚A and b = 20 ˚A

Energy (eV)	Randall D. Knight (2007)	Lima (2020)	This Work N = 5	This Work N ≥ 30	Relative error w.r.to (Knight, 2007)
E_1	0.068	0.0666	0.0664	0.0663	0.025
E_2	0.263	0.2588	0.2650	0.2620	0.003
E_3	0.583	0.5582	0.5758	0.5774	0.013
E_4	0.949	0.9168	-	0.9818	0.034

Conclusions

In the realm of undergraduate quantum mechanics education, we have illuminated a path where the versatile and freely accessible software, SMath Studio, serves as a conduit for applying a sophisticated matrix method to the numerical unraveling of the one-dimensional finite square well potential nestled within the expansive embrace of its infinite counterpart. This digital foray, facilitated by the intuitive design of the SMath Studio worksheets, empowers students to navigate the complexities of computer-assisted solutions without the prerequisite of programming expertise. This innovative educational strategy not only demystifies the foundational principles of quantum mechanics but also paves the way for an adventurous exploration of more intricate quantum landscapes. Students are thus equipped to extend this methodology to dissect the time-independent Schrödinger equation across a spectrum of one-dimensional potentials, from the harmonious dance of particles in a harmonic oscillator potential, familiar in the introductory narratives of quantum mechanics, to the more complex choreographies of the anharmonic oscillator and the finite double-square well potentials. Venturing further into this quantum tapestry, students are encouraged to delve into the construction of larger matrices, assembling n×n squares from a tapestry of linearly independent eigenvectors, where n exceeds the quintet. This mathematical expedition not only broadens

their understanding of quantum mechanics but also invites them to probe the depths of potential wells, seeking the elusive threshold beneath which bound states emerge as quantum certainties, adding a rich layer of comprehension to their academic voyage through the quantum realm.

Data Availability

The data used and analyzed for the outcomes reported in the manuscript are available from the corresponding author on reasonable request.

Funding

Not Applicable.

Declarations

Ethical Statement

We complied with all required ethics for data collection and analysis for the outcomes we have reported in this manuscript.

Informed Consent

Not Applicable.

Conflict of Interest

The authors declare no competing interests.

Consent to Publish

Not Applicable.

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