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Solution of the Time-Independent Schrödinger Equation for the Rosen–Morse Potential by Using the Galerkin Method

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Abstract

This study presents a numerical solution to the time-independent Schrödinger equation (TISE) for the Rosen-Morse potential using the Galerkin method. The Rosen-Morse potential, commonly used in atomic and molecular physics, has known analytical solutions under certain conditions. By transforming the TISE into a Jacobi differential equation, the analytical wave function and energy levels can be derived. However, analytical solutions are limited to ideal cases, highlighting the need for numerical methods in more general scenarios. The Galerkin method is implemented by expanding the wave function using Sine basis functions and projecting the TISE onto this basis. The resulting eigenvalue problem is solved by constructing the Hamiltonian matrix from kinetic and potential energy operators. Numerical results from the Galerkin method are compared with analytical solutions using graphical analysis, percentage error (% error), and statistical tests, including the Mann-Whitney U test. The results demonstrate that the probability densities obtained using the Galerkin method closely approximate the analytical solution. This is visually evident from the overlapping of probability density plots from both methods. The percentage error of the probability densities is below 1 %, entirely. Furthermore, the Mann–Whitney U test yields a p-value less than 0.05, indicating that the differences between the two sets of probability densities are statistically insignificant at the 95% confidence level. These findings highlight the Galerkin method's effectiveness and accuracy as a robust numerical tool for solving the TISE with the Rosen-Morse potential.

Introduction

The Schrödinger equation is one of the fundamental pillars of quantum mechanics, particularly in describing the dynamics of closed quantum systems. This equation, especially

in its time-independent form (TISE), is frequently employed to analyze stationary states and the discrete energy spectrum of particles within a given potential. However, modern developments in quantum mechanics have introduced various alternative frameworks to gain a more comprehensive understanding of quantum phenomena. For example, the Schrödinger picture emphasizes the time evolution of the wavefunction, whereas the Heisenberg picture transfers the time dependence to physical operators, which proves useful in analyzing dynamical systems and in the formulation of quantum field theory. On the other hand, the interaction picture is widely used in perturbation theory and in studying interacting systems, such as those encountered in quantum electrodynamics. Moreover, in open quantum systems that interact with external environments, approaches such as the master equation become essential. These frameworks describe the non-unitary evolution of the quantum state by incorporating effects such as decoherence and dissipation phenomena not accounted for by the standard Schrödinger equation. Recognizing the diversity of these perspectives, the use of the TISE in this study serves as a controlled analytical starting point, laying the foundation for further exploration of quantum dynamics and possible extensions into alternative frameworks depending on the physical context of the system under investigation. Solving the TISE allows us to obtain the wave function and energy of a particle in various potential forms. One particularly interesting potential to study is the Rosen-Morse potential, which has applications in various fields such as atomic physics, molecular physics, and other quantized systems [1][2][3] [4][5]. This potential can also be used to model interactions in two-level quantum systems, potential barriers with asymptotic characteristics, and asymmetric potential well profiles. The Rosen–Morse potential incorporates exponential and hyperbolic features that are not present in many classical potential forms.

Compared to classical potentials such as the Coulomb potential, the harmonic oscillator, and the infinite square well, which possess well-known analytical solutions and ideal symmetries. The Rosen–Morse potential offers a more complex and flexible structure due to its asymmetry and its dependence on shape parameters. Furthermore, in comparison with other potential forms such as the delta potential (Dirac delta potential), the finite square well, the Morse potential, and the Pöschl–Teller potential, the Rosen–Morse potential remains distinctive in its ability to smoothly transition between a barrier and a well structure simply by adjusting a few parameters. The complexity of the Rosen–Morse potential reflects more realistic physical systems, especially in non-ideal environments or long-range interactions where symmetry is broken. In many practical scenarios, real-world quantum systems do not conform to simple potential models. Thus, the development of numerical methods to solve the TISE for more intricate potentials like Rosen–Morse is of significant importance. In recent decades, computational quantum mechanics has seen substantial progress in the development of numerical methods to address such challenges. Finite difference methods (FDM), finite element methods (FEM), spectral methods, and variational approaches have all been employed with increasing sophistication to solve quantum systems. These techniques enable researchers to address nontrivial potentials and boundary conditions with improved accuracy and computational efficiency. Among these, spectral methods—including Galerkin-based formulations, offer exponential convergence for smooth problems and are particularly effective for problems with well-behaved boundary conditions. Consequently, this research also serves as a platform to test and evaluate the effectiveness of a spectral-based numerical approach, namely the Galerkin method, in handling quantum systems with higher potential complexity.

Analytical methods are often used to solve the Schrödinger equation, but these methods can only be applied to specific cases with potential forms that allow for exact solutions. Although analytic methods provide exact and accurate solutions, they exhibit several significant limitations, particularly in their application to complex potential forms or systems involving multiple variables. These methods are typically restricted to specific types of potentials (such as the infinite square well, harmonic oscillator, the Coulomb potential, and similar well-studied ones). Analytic approaches also rely heavily on special functions (e.g., Jacobi, Legendre, or hypergeometric functions), which can be difficult to compute and analyze. In contrast, numerical methods such as the Galerkin method, the Finite Difference Method (FDM), the Shooting Method, and the Variational Method offer greater flexibility, can handle a wider range of potential functions, and are generally easier to implement, although the results are approximate in nature. Therefore, numerical methods serve as an important alternative approach to solving the Schrödinger equation for various types of potentials. In this study, the Galerkin method is employed as a numerical approach to solving the time-independent Schrödinger equation with the Rosen-Morse potential. The Galerkin method is known as one of the finite element-based approximation techniques that effectively handle various types of differential equations [6][7] [8] [9] [10] . Unlike a standard expansion method, which directly approximates the solution via truncated basis functions and determines coefficients without necessarily enforcing residual orthogonality, the Galerkin method requires the residual to be orthogonal to all basis functions in the chosen subspace. This projection property leads to a more rigorous and systematically derived set of algebraic equations, produces a symmetric and well-conditioned system (for orthonormal bases), and generally yields higher accuracy and convergence for smooth potentials such as Rosen–Morse.

This study is expected to provide further insights into the application of the Galerkin method in quantum mechanics and to enhance the understanding of numerical solutions to the Schrödinger equation. Additionally, the obtained results can serve as a reference for the development of other, more efficient and accurate numerical methods for solving differential equations in quantum physics and related fields.

Theory and Calculation

Analytical Solution to the TISE for the Rosen-Morse Potential

The time-independent Schrödinger equation (TISE) is expressed as [11][12] [13][14]:

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

where ψ(x) is the wave function, E is the eigen energy, $\hbar$ is the reduced Planck constant, m is the mass of the particle, V(x) is the potential energy, and x denotes the position of the particle. The Rosen–Morse potential V(x) is given by [15]:

$$V(x) = 2\lambda\, tanh(\alpha x) - \frac{s(s+1)}{cosh\,(x)^2} \quad (2)$$

thus, (2) becomes:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + 2\lambda\, tanh(\alpha x) - \frac{s(s+1)}{cosh\,(x)^2}\psi(x) = E\psi(x) \quad (3)$$

where λ is the potential asymmetry parameter, α denotes potential width and s is a parameter proportional to the potential depth. Increasing s makes the well deeper and narrower. The shape of the potential energy curve V(x) for several values of λ and α = 1 is shown in Figure 1.

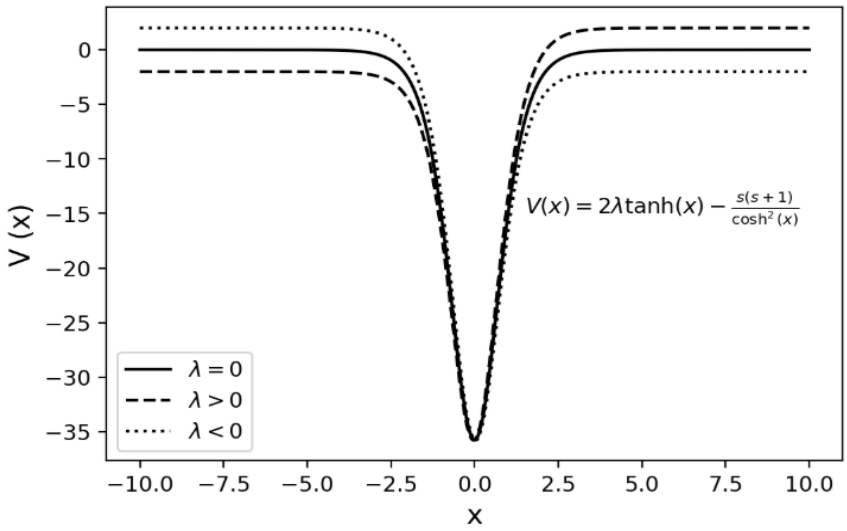


Figure 1. Rosen-Morse potential

The normalized bound-state solutions for this equation (3) can be expressed directly in terms of x [15]:

$$\psi_{s,\lambda}(n;x) = M_n cosh^{-(s-n)}(x)\, e^{(-\frac{\lambda x}{s-n})}\, P_n^{(\mu,\nu)}(tanh(x)) \tag{4}$$

M_n is a normalization constant and $P_n^{(\mu,\nu)}$ denotes the Jacobi polynomial [16][17][18][19]. The corresponding energy levels, on the other hand, are given by:

$$E_n = -(s-n)^2 + \frac{\lambda^2}{(s-n)^2} \tag{5}$$

This solution is valid for quantum numbers n = 0,1, …, n_{max}, where $n_{max} < s - \sqrt{\lambda}$.

Solving the TISE for the Rosen-Morse Potential by Using the Galerkin Method

The Galerkin method is a numerical approach that can be employed to solve the TISE with a potential defined over an infinite domain, such as the Rosen-Morse potential. The following are the steps of the Galerkin approach used to solve the TISE for the Rosen-Morse potential:

a) Define the domain $x \in [-L, L]$ sufficiently large such that the bound-state wavefunction decays to zero at the boundaries (e.g., L~10).
b) Use an orthonormal basis over this interval, for example, sine $\phi_n(x)$ and cosine $\varphi_n(x)$ function [20][21][22][23][24] which satisfy the boundary conditions $\phi_n(-L) = \phi_n(L) = 0$.

$$\phi_n(x) = \frac{1}{\sqrt{L}} \sin\left(\frac{n\pi(x+L)}{2L}\right) \quad (6)$$

$$\varphi_n(x) = \frac{1}{\sqrt{L}} \cos\left(\frac{(2n-1)\pi(x+L)}{2L}\right) \quad (7)$$

c) Construct the Hamiltonian matrix H, defined as:

$$H_{ij} = \int_{-L}^{L} \phi_i(x) \left[-\frac{d^2}{dx^2} + V(x)\right] \phi_j(x) dx \quad (8)$$

This matrix is computed by evaluating the kinetic component (T_{ij}) and potential energy one (V_{ij}):

$$T_{ij} = \int_{-L}^{L} \phi_i(x) \left(-\frac{d^2}{\partial x^2}\right) \phi_j(x)\, dx = \left(\frac{n\pi}{2L}\right)^2 \quad (9)$$

$$V_{ij} = \int_{-L}^{L} \phi_i(x)\, V(x) \phi_j(x) dx \quad (10)$$

where V(x) is the Rosen–Morse potential as defined in (2). Eq. (10) is evaluated numerically. The spatial domain x ∈ [−L, L] is discretized into N_x equally spaced grid points (in our implementation, L=10 and N_x =1001). The basis functions $\phi_i(x)$ and $\phi_j(x)$, as well as the Rosen–Morse potential V(x), are computed at each grid point. The integral is then approximated using the composite trapezoidal rule: $V_{ij} = \sum_{k=1}^{Nx} \phi_i(x_k) V(x_k) \phi_j(x_k)\, \Delta x$, where $\Delta x = \frac{2L}{Nx-1}$ is the grid spacing.

d) The wavefunction expressed as:

$$\psi(x) = \sum_{i=1}^{N} c_i \phi_i(x) \quad (11)$$

N is the total number of basis functions, c_i are the expansion coefficients and $\phi_i(x)$ the chosen basis function. Coefficients c_i can be reached by solving the eigenvalue equation:

$$\mathbf{Hc} = E\mathbf{c} \quad (12)$$

E and **c** are the eigenvalues (energy levels) and the corresponding basis coefficients (eigenvectors), respectively.

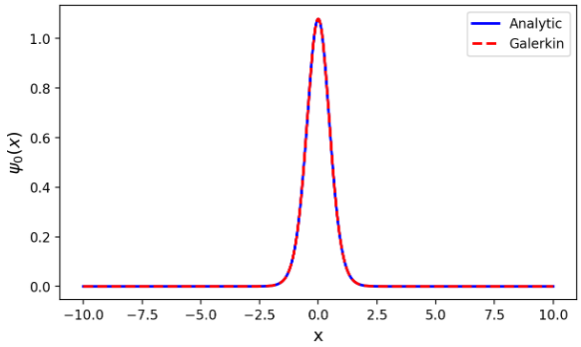
In summary, the Galerkin method is a projection technique in which the exact solution of the time-independent Schrödinger equation (3) is approximated within a finite-dimensional subspace spanned by a chosen set of basis functions. The wavefunction is expressed as a linear combination of these basis functions, and this approximate form is substituted into equation (3). The difference between the left-hand and right-hand sides of equation (3), known as the residual, is then required to be orthogonal to each basis function in the subspace. This orthogonality condition transforms the continuous differential equation into a discrete matrix eigenvalue problem of the form **H c** = E **c**, where the matrix elements H_{ij} are computed from the kinetic and potential energy integrals. The eigenvalues E provide the approximate energy levels, and the eigenvectors **c** yield the corresponding expansion coefficients for the approximate wavefunctions. Increasing the number of basis functions systematically improves the accuracy, and in the limit of an infinite basis set, the exact solution is recovered.

Experimental Method

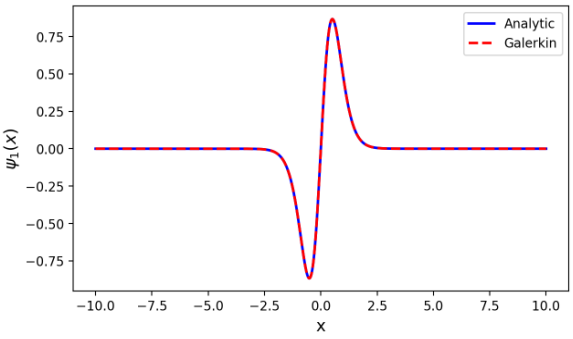
Initially, a flowchart was designed based on steps (a) through (e) as mentioned earlier. Following the design of the flowchart, the next step involved implementing the flowchart into program code. The programming language used in this study was Python [25]. The computer utilized for this research was an HP laptop with the following specifications: Intel Core i7 processor, 16 GB RAM, and an 8 GB GPU. The complete source code and flowchart for the solution of the TISE by the Galerkin method can be obtained upon request by contacting the author via email.

Result and Discussion

The solutions of the TISE for the Rosen-Morse potential using the Galerkin method and the analytical approach are presented in the form of wave functions and energy levels. The wave functions, $\psi_n(x)$, for quantum numbers n = 0, 1, …, 4, are presented in Figure 3. In this study, each wave function $\psi_n(x)$, was sampled using 1001 data points (N_x) uniformly distributed over the domain L= [−10,10]. A total of 700 basis functions (N) were employed.



(a)



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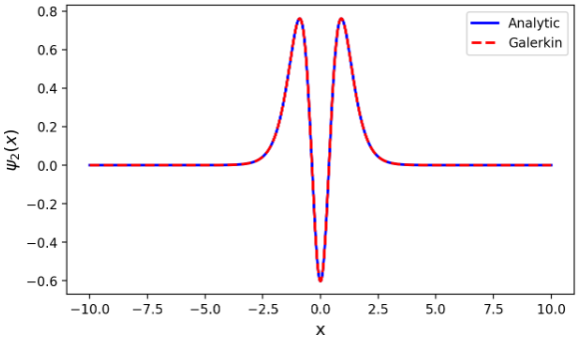

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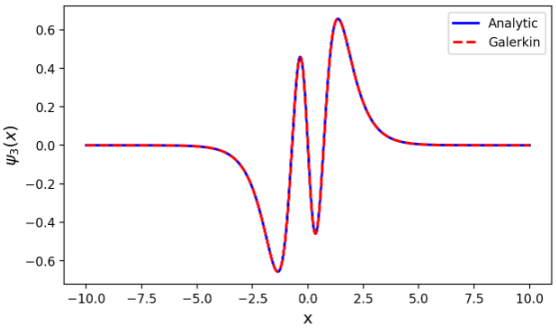

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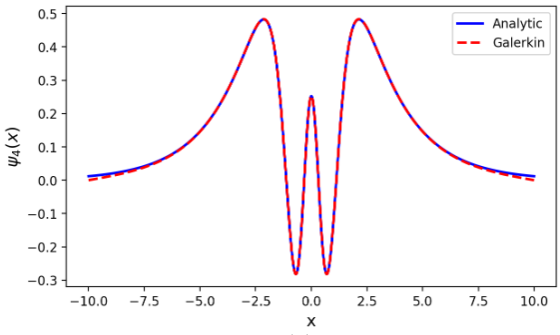


(e)

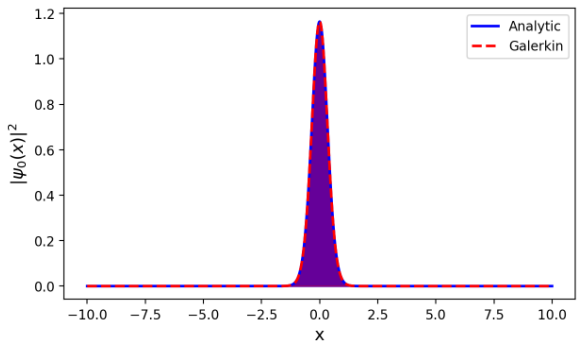
Figure 3. Plotting of (a) $\psi_0(x)$, (b) $\psi_1(x)$, (c) $\psi_2(x)$, (d) $\psi_3(x)$ and (e) $\psi_4(x)$

Meanwhile, the energy levels En are presented in Table 1. As shown in Table 1, the relative error is negligible (≈0) for low-energy states (i.e., small n). The error becomes noticeable starting from n=4, but remains below 0.12%, demonstrating the excellent convergence of the Galerkin method.

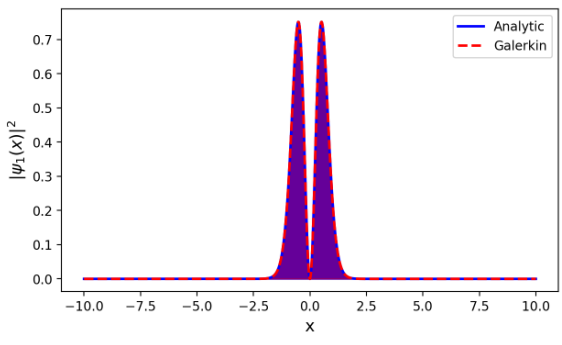
Table 1. Energy levels, E_n - Analytical vs. Galerkin

n	E_n (analytical)	E_n (Galerkin)	Relative Error (%)
0	-20.250000000000	-20.250000000000	0.000000000000
1	-12.250000000000	-12.249999999999	0.000000000008
2	-6.250000000000	-6.250000000000	0.000000000000
3	-2.250000000000	-2.249999999943	0.0000000025337
4	-0.250000000000	-0.249709809824	0.116076070400

Figure 3 presents the wave function $\psi_n(x)$ obtained from the Analytic and Galerkin methods, depicted by blue and red curves, respectively. Figure 4, on the other hand, shows the probability density $|\psi_n(x)|^2$ obtained from both methods. Visually, it is evident that the curve produced by Galerkin method coincides with the Analytic one. Ideally, both curves should overlap, indicating that the analytical solution matches or at least closely approximates the numerical one[26][27].



(a)



(b)

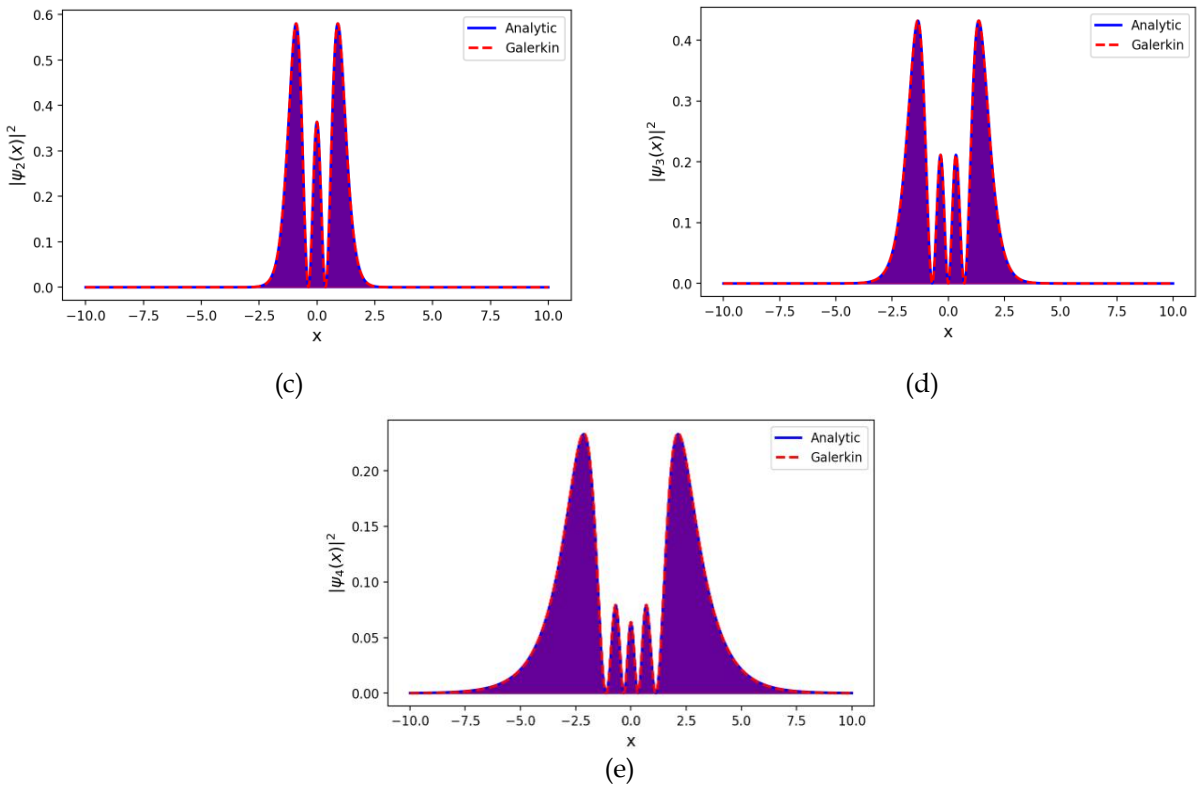


Figure 4. Plotting of (a) $|\psi_0(x)|^2$, (b) $|\psi_1(x)|^2$, (c) $|\psi_2(x)|^2$, (d) $|\psi_3(x)|^2$ and (e) $|\psi_4(x)|^2$

However, this visual observation requires quantitative validation. In order to quantitatively compare the computed results of $|\psi_n(x)|^2$ obtained from the Galerkin and analytical methods, the percentage error (% error) and the Mann-Whitney U test (hereafter referred to as the U test) were employed[28]. The first quantitative comparison is the percentage error of the probability densities $|\psi_n(x)|^2$ obtained from both methods, presented in the following Table 2.

Table 2. Percentage error $|\psi_n(x)|^2$ - Analytical vs. Galerkin

n	Percentage error (%)
0	0.000000000000
1	0.000000000002
2	0.000000000000
3	0.000000027077
4	0.256905327729

As shown in Table 2, the entire percentage errors are very small, smaller than 1 %, indicating that the results obtained from both methods are nearly identical. The second one is the U test. The U test was applied as a non-parametric approach that does not require the assumption of normal data distribution. This choice is particularly appropriate, since the quantum probability density functions $|\psi_n(x)|^2$ obtained from both analytical and Galerkin methods, as confirmed by the following Shapiro–Wilk test, do not exhibit normal distribution characteristics. Examples of the Shapiro-Wilk normality test results for n = 3 and n = 4 are presented in Tables 3 and 4, respectively, with a significance level (α) of 0.05.

Table 3. Saphiro-Wilk Test for $|\psi_3(x)|^2$

Method	Saphiro-Wilk statistic	p-value
Analytic	5.36e-01	2.80e-45
Galerkin	5.36e-01	2.80e-45

Table 4. Saphiro-Wilk Test for $|\psi_4(x)|^2$

Method	Saphiro-Wilk statistic	p-value
Analytic	7.31e-01	2.43e-37
Galerkin	7.31e-01	2.43e-37

From Tables 3 and 4, it can be observed that all p-values are less than 0.05. Therefore, it can be concluded that the distributions of $|\psi_3(x)|^2$ and $|\psi_4(x)|^2$ obtained from the Analytical and Galerkin methods do not follow a normal distribution. Similarly, the results of the normality tests for n = 0, 1, and 3 also yield p-values less than 0.05, leading to the conclusion that the data do not follow a normal distribution. The results of the U test between the Galerkin and Analytical methods, with a significance level (α) of 0.05, are presented in Table 5.

Table 5. U Test - Analytical vs. Galerkin

n	U Statistic	p-value
0	4.92e+05	2.54e-01
1	5.00e+05	4.83e-01
2	5.00e+05	4.69e-01
3	4.99e+05	4.44e-01
4	4.88e+05	1.57e-01

From Table 5, it can be observed that all p-values are greater than 0.05. Therefore, it can be concluded that the computed values of $|\psi_n(x)|^2$ (for n = 0, 1, ..., 4) obtained using the Galerkin method are statistically equivalent to those obtained using the analytical method, with a 95% confidence level. In other words, we are 95% confident that the results from both methods do not differ significantly.

Conclusion

The Galerkin method was shown to produce probability density functions $|\psi_n(x)|^2$ that closely match the analytical solutions. The percentage error was shown to be less than 1%, indicating high numerical accuracy. Statistical analysis using the Mann-Whitney U test confirmed no significant differences between the two methods at the 95% confidence level. Therefore, the Galerkin method is validated as an accurate numerical approach for solving the TISE involving the Rosen-Morse potential.

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