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Simulation of Time Independent Schrödinger Equation for Finite Potential Well Using the Graphical Solution Method

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ABSTRACT

This paper investigates applying the approximate method; Graphical Solution Method (GSM), to theoretically solve the Time Independent Schrödinger Equation (TISE) in one dimension for a finite square well using MATLAB. With just few lines of MATLAB coding, calculating and plotting accurate eigenvalues (energy), eigenvectors (wave functions) and the bound eigenstates are possible for the finite square well of a negative potential (depth of the well) of -400 eV and a well width of 0.1 nm for an electron confined to this quantum well. These eigenvalues, eigenvectors and eigenstates are obtained and discussed. The found energy eigenvalues and states are discrete and yield physical acceptable solutions. The even and odd solutions of the TISE are also considered. The graphical solutions for the finite potential well are shown. The locations of discrete eigenvalues for even and odd solutions are also presented. These eigenvalues are tested confirming the correct eigenfunctions. The precision of these solutions depend on well width L and on the interval dx used to integrate the equation. Exact analytical solutions for this case are obtained and compared with results from the GSM. The accuracy and the convergence of the numerical results are easily checked. The results showed that the GSM can be considered as a suitable mean for determining the one dimensional solutions for the finite square well.

محاكاة معادلة شرودنجر غير معتمدة على الزمن لبئر الجهد المحدود باستخدام طريقة الحل البياني

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الكلمات المفتاحية:
معادلة شرودنجر غير معتمدة على الزمن
بئر مربع محدود
طريقة الحل البياني
القيم الذاتية للطاقة
دوال ذاتية

الملخص

هذا الورقة تتحقق نظريا من تطبيق طريقة التقريب، طريقة الحل البياني(GSM) ، لحل معادلة شرودنجر غير معتمدة على الزمن (TISE) في بعد واحد لبئر الجهد المحدود باستخدام الماث لاب . (MATLAB) بفقط عدد قليل من برامج الماث لاب، كان من الممكن حساب ورسم القيم الذاتية الصحيحة (طاقة) ، المتجهات الذاتية (دوال الموجه)، والحالات الذاتية المقيدة لبئر مربع محدود لجهد سالب (عمق البئر) بقيمة -400 eV وعرض البئر بقيمة 0.1 nm لإلكترون محصور في هذا البئر الكمي. تم مناقشة هذه القيم الذاتية، المتجهات الذاتية والحالات الذاتية المتحصل عليها. القيم الذاتية وحالات طاقة المتحصل عليها منفصلة وتنتج حلول فيزيائية مقبولة. ايضا تم حساب الحلول الزوجيه والفردية لمعادلة شرودنجر غير معتمدة على الزمن. تم توضيح الحلول البيانية للبئر محدود الجهد. مواقع القيم الذاتية المنفصلة للحلول الزوجية والفردية ايضا تم عرضها. تم اختبار هذه القيم الذاتية لتأكيد الدوال الذاتية الصحيحة. دقة هذه الحلول يعتمد على عرض البئر L والفترة dx المستخدمة لتكامل المعادلة. تم ايجاد الحلول التحليلية الدقيقة لهذه الحالة ومقارنتها مع نتائج طريقة الحل البياني. (GSM) دقة وتقارب النتائج العددية يمكن فحصها بسهولة. النتائج بينت ان طريقة الحل البياني يمكن اعتبارها وسيلة مناسبة لحساب حلول البعد الواحد للبئر المربع المحدود.

Introduction

Historically, Quantum Mechanics is considered to have two independent formulations; Matrix mechanics and Wave Mechanics.

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The development of matrix mechanics in 1925 was credited to Heisenberg for his theory and the description of atomic structure starting from spectral lines. The discovery of wave mechanics was attributed to Schrödinger who suggested it by generalizing de-Broglie postulation in 1926. Wave mechanics described the dynamics of microscopic matter by means of a wave equation called Schrödinger Equation. Erwin Schrödinger developed this linear partial differential equation of second order to explain the wave nature of matter and particle associated to wave [1-5]. This equation is similar to the wave equation in optics which is based on the assumption that a particle behaves as a wave. This equation attracted the attention of researchers since its formulation [3, 6]. The solution of the Schrodinger equation is still a fundamental part of many disciplines of science [7-17]. Semiconductor devices characterization and nanostructures are examples of this [18]. The solution of the Schrödinger Equation contains both wave function (ψ) and the energy (E) of the particle under consideration. The wave function ψ is most important because when the wave function is obtained, the particle's parameters can be identified. Parameters such as the probability of finding the particle in a certain region at a position x, within a region of length dx, at a particular instant of time t can be specified by the absolute square of Ψ, $|\psi(x,t)|^2$. The energy of particle, E, depends on the potential V and the boundary conditions. E and V are very important parameters since both are constraints on the particle. These parameters are either quantized or continuous [2].

Theoretical Considerations

Subject to its dependency on time, Schrödinger equation can be categorized as either Time Dependent Schrödinger Equation (TDSE) or Time Independent Schrödinger Equation (TISE) [2]. There are numerous applications of quantum well models in, for example, nanostructures and other fields [18]. For the case considered in this paper, TISE has the following form:

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

This equation is to be solved according to a number of some selected variables whose input values are assigned initially, such as the width, depth and the number of data points for the case of finite square well. Even though, there are previous attempts to solve this equation using iterative method, e.g. [19-21], these may be lengthy and time consuming. To attempt a quicker routine, the Graphical Solution Method (GSM) using MATLAB simulations is used and applied to the finite square well in this paper. The finite square well is defined as in Figure 1 showing the values of *x* inside and outside with a length *L*.

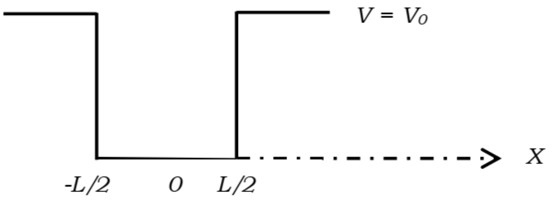


Figure 1 The finite square well.

The Schrödinger equation inside the finite well is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi. \quad for\ -1/2 \le x \le 1/2. \quad (2)$$

Rewriting it as:

$$\frac{d^2\psi}{dx^2} + K_1^2\psi = 0 \quad (3)$$

Where

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad (4)$$

The finite well, shown in Figure 1, has a depth of V_0. Outside the well, the Schrödinger equation is:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi. \quad for|x\,| \ge L/2 \quad (5)$$

For values of energy *E* less than the depth V_0, the Schrödinger equation for the region outside the well is:

$$\frac{d^2\psi}{dx^2} - K_2^2\psi = 0 \quad (6)$$

Where

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (7)$$

E less than V_0 implies that (V_0 - *E*) is positive and that is K_2 is a real number. Inside the well, TISE has even and odd solutions of the form:

$$\psi_{even} = \begin{cases} Aexp(K_2x), x \le -L/2 \\ Bcos(K_1x), -L/2 < x < L/2, \\ Dexp(-K_2x). x \ge L/2 \end{cases} \quad \psi_{odd=} \begin{cases} Aexp(K_2x), x \le -L/2 \\ Csin(K_1x), -L/2 < x < L/2 \\ Dexp(-K_2x). x \ge L/2 \end{cases}$$

where:

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}}, \qquad K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

(a) Even solutions

$$\psi(x) = Bcos(K_1x), \quad for - L/2 \le x \le L/2 \quad (8)$$

$$\psi(x) = D\exp(-K_2x), \quad for\ x \ge L/2 \quad (9)$$

For the solution to be continuous at $x = L/2$, the following form is found:

$$B\ cos\left(\frac{K_1L}{2}\right) = D\ exp\left(-\frac{K_2L}{2}\right) \quad (10)$$

Likewise, the derivative of the solution has to be also continuous at $x = L/2$ as in this equation:

$$-BK_1sin\left(\frac{K_1L}{2}\right) = -D\ K_2exp\left(-\frac{K_2L}{2}\right) \quad (11)$$

To remove the constants *A* and *B* from the above equations, Eq. (11) is divided by Eq. (10) :

$$\tan\left(\frac{K_1L}{2}\right) = \frac{K_2}{K_1} \quad (12)$$

(b) Odd Solutions

$$\psi(x) = Csin(K_1x), \ \ for - L/2 \le x \le L/2 \quad (13)$$

$$\psi(x) = D\exp(-K_2x), \ \ for\ x \ge L/2 \quad (14)$$

Again, the solution has to be continuous at $x = L/2$ yielding:

$$C\ sin\left(\frac{K_1L}{2}\right) = D\ exp\left(-\frac{K_2L}{2}\right) \quad (15)$$

Again, the derivative of the solution has to be continuous at $x = L/2$ through this equation:

$$C\ K_1cos\left(\frac{K_1L}{2}\right) = -DK_2exp\left(\frac{K_2L}{2}\right) \quad (16)$$

Dividing Eq.(16) by Eq. (15) gives:

$$-\cot\left(\frac{K_1L}{2}\right) = \frac{K_2}{K_1} \quad (17)$$

Eqs. (12) and (17) have no analytical solution and must be solved using numerical methods. Substituting Eq. (7) into Eq. (12) and Eq. (17) yields:

$$\tan\left(\frac{K_1l}{2}\right) = \sqrt{\frac{2mVo}{\hbar^2K_1^2} - 1}, \quad (18)$$

$$-\cot\left(\frac{K_1L}{2}\right) = \sqrt{\frac{2mVo}{\hbar^2K_1^2} - 1} \quad (19)$$

Eqs. (18) and (19) can be expressed in terms of the dimensionless variables as follows:

$$\xi = \frac{K_1L}{2} = \frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}, \qquad \beta = \frac{L}{2}\sqrt{\frac{2mV_0}{\hbar^2}} \quad (20)$$

One gets:

$$\tan(\xi) = \sqrt{\frac{\beta^2}{\xi^2} - 1}, \qquad n = 1,3,5,\ldots \quad (21)$$

$$-\cot(\xi) = \sqrt{\frac{\beta^2}{\xi^2} - 1}, \qquad n = 2,4,6,\ldots \tag{22}$$

These equations can be solved using the Graphical Solution Method (GSM). The energies for bound states are determined by plotting the left-and right-hand sides of Eq. (21) and Eq. (22) and by finding the point where the curves intersect with each other. There are two basic possibilities for the energy E and the potentials depending on the shape of the well: That is:

1. If $E > V_0$ (unbound states), the wave number k has the general form $\sqrt{2m(E-V_0)/\hbar^2}$. Inside the well, k is equal to $\sqrt{2mE/\hbar^2}$, and outside the well it is equal to $\sqrt{2m(E-V_0)/\hbar^2}$. The wave function is an oscillatory function inside and outside the well, because the wave number k is real everywhere and large inside the well, thus the wavelength is short.
2. In finite potential wells, the particle is not exactly confined where its wave position may spread into classically forbidden areas. Therefore, the particle can be everywhere since the wave function extends infinitely on both directions; hence the name unbound states. This case is not considered in this study.
3. If $0 < E < V_0$ (bound states), the wavenumber is $\sqrt{2mE/\hbar^2}$ inside the well, while outside the well it is equal to $\sqrt{2m(E-V_0)/\hbar^2}$ or $\sqrt{2m(V_0-E)/\hbar^2}$ (imaginary case). Therefore, inside the well the wave function is an oscillatory function while outside the well the wave function is an exponential decaying function; otherwise the wave function would diverge at $x = \pm\infty$. Studying such cases is the aim of this paper.

It is most important to find the energies and states, which should be discrete, by solving the TISE for a number of arbitrary potentials. These values of energy should yield physical acceptable solutions, i.e the wave function at the $x = \pm\infty$ must approach to zero. That is $(\psi(x_{min}) = \psi(x_{max}) = 0)$. How precise these solutions are depend on the width L of the well and on the interval dx used to integrate the equation.

Results and Discussion

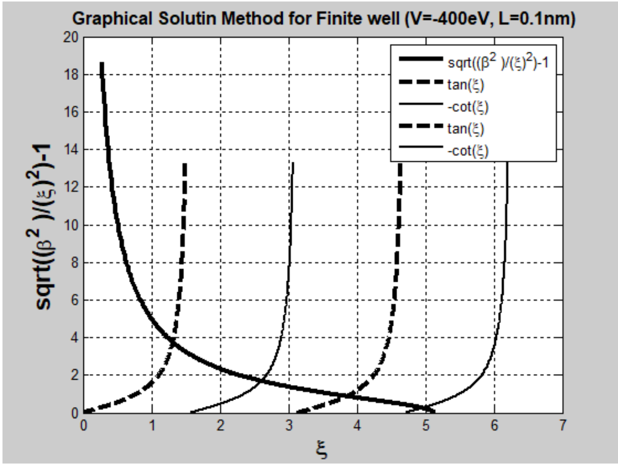
In this part of the work a negative potential (depth of the well) V = -400 eV, and the width of the well L= 0.1 nm are chosen and simulated using codes in [22]. The value of β^2 for an electron confined to this quantum well with these parameters can be found as:

$$\beta^2 = \frac{mV_0L^2}{2\hbar^2}$$

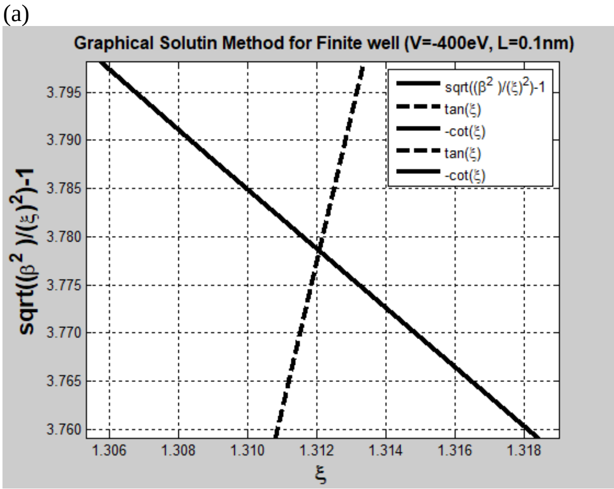
$$\beta^2 = \frac{5.6875\times10^{-12}\times400\times(1\times10^{-10})^2}{2\times(0.658\times10^{-15})^2} = 26.3$$

$$\beta = \sqrt{26.3} = \pm5.13$$

Before plotting the left-and right hand sides of Eqs. (21) and (22), it is to be noted that the common right-hand side of the two equations becomes infinite at $\beta = 0$ and assumes an imaginary values for ξ greater than $\beta = 5.13$. The right- hand sides of the equations can be plotted from a value slightly greater than $0 \rightarrow \beta$, and the left-hand sides of the two equations must be plotted in segments because *tan*(ξ) becomes infinite at $\pi/2$ and $3\pi/2$, where *cot*(ξ) becomes infinite at π and $2\pi = 6.28$. The points of intersections for left- and right-hand sides of Eqs. (21) and (22) are found by the MATLAB codes [22]. The first line of the MATLAB program defines the value of β, the second line of the program then produces a vector, ξ, consisting of value of ξ for 400 equally-spaced points between 0.275 and β. The next line of code produces a vector y, having the values of common right-hand sides of equations (21) and (22), at the points ξ. The fourth line of program produces a vector, ξ_1, with value of 0.0 to a point slightly before $\pi/2$ where the tangent function is singular, and the next line defines a vector y_1, giving the values of tangent at those values of ξ. Similarly, ξ_2 is a vector with the value of ξ between $\pi/2$ and slightly before π, and ξ_3 is a vector with values of ξ between π and slightly before $3\pi/2$. y_2 yields the value of the negative of the cotangent for the points ξ_2 , while y_3 gives the value of tangent for points ξ_3. Finally the last line of the program produces the plot. Figure 1 (a,b) shows the graphical solution for finite potential well where $\beta = 5.13$. This figure is used to estimate the value of ξ for the first intersection of the curves.



(a)



(b)

Figure 1 (a) Location of discrete eigenvalues for even and odd solutions using GSM. (b) The part of Figure (a) used to estimate the value of ξ for first intersection of the curves.

The procedure for getting the intersection point is as follows:
The energy of the even solutions correspond to the points where the tangent curve intersects the curve corresponding to the right-hand side of the equations, while the energy of the odd solutions correspond to the points where the negative of the cotangent intersects the curve corresponding to the right-hand side of the equations. The value of ξ for the first intersection point can be estimated, as shown in Figure 1 (b), to be $\xi = 1.3121$. Table 1 shows the even and odd solutions of the functions considered.

Table 1: Even and odd solutions

Even Solution	Odd solution
1.3121	2.608
3.8602	4.970

The values of the energy for particular values of ξ can be calculated by using definition $\xi = K_1 l/2$ to derive the following equation:

$$E = \frac{2\hbar^2\xi^2}{m_e L^2} + V_0 \tag{23}$$

Substituting $\xi_1 = 1.3121$, ħ=0.658 x 10^{-15} eV.s , m_e = 5.6875 x 10^{-12} eV/C^2, width L= 0.1 *nm*, and the depth V_0=-400 eV into equation (23) gives:
E_1= 26.21 – 400 = -373.788 eV.
Similarly, the values of energy E corresponding to the other three intersections are estimated to be:

E_2 = 103.5618 – 400 = - 296.438 eV,
E_3 = 226.884 – 400 = - 173.116 eV, and
E_4 = 376.107 – 400 = - 23.893 eV.

The wave functions for these four states are denoted by ψ_1, ψ_2, ψ_3, and ψ_4. Figure 2 shows the even and odd bound solutions of an electron in a finite well. After obtaining the energy eigenvalues from the GSM, these eigenvalues are tested to check that they yield the correct eigenfunctions, i.e. physically acceptable solution (wave function converges to zero at boundary conditions). From Figure 2, it can be seen that the correct wave function (physically acceptable solution) is obtained from the three first eigenvalues. However, the last eigenvalue gave an invalid wave function, because at end of the well the wave is not equal to zero. This means that the last value for energy eigenvalue at n = 4, E_4= - 23.893 eV using GSM corresponds to the end value of wave function $\psi_4(x_{max}) = -4.41 \times 10^4$ near the boundary conditions. The reason is that the fourth intersection point is not very accurate, $\xi = 4.965$. The intersection yields the same result for $\xi = 4.989$ at E_4 = -21.325 eV corresponding to the end wave function $\psi_4(x_{max})$= - 6.03 x 10^3.

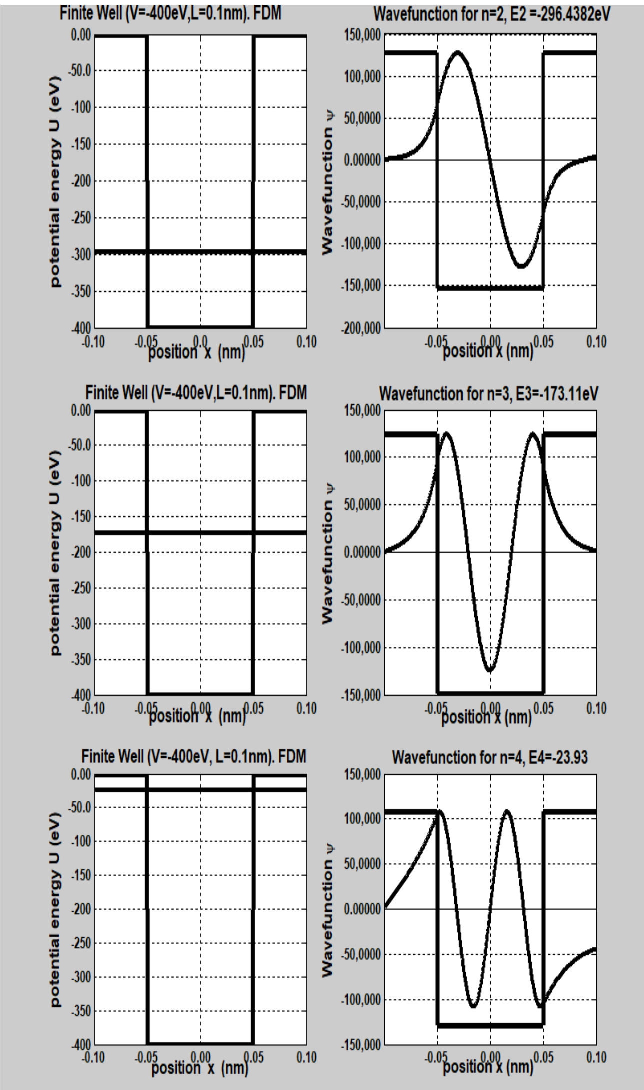


Figure 2 The even and odd bound solutions of an electron in a finite well.

Conclusion

In this paper an attempt an attempt is made to find the energy eigenvalues and wave functions for the particle inside the finite square well potential by solving time independent Schrodinger equation (TISE) via the Graphical Solution Method using MATLAB. Accurate eigenvalues (energy), eigenvectors (wave functions) and the bound eigenstates were calculated and plotted for a negative potential of -400 eV and a width of 0.1 nm for an electron confined to this quantum well. The found energy eigenvalues and states were discrete and yield physical acceptable solutions. The locations of discrete eigenvalues for even and odd solutions were also presented. Exact analytical solutions for this case were found and compared with results from the GSM. The accuracy and the convergence of the numerical results are easily checked.

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