A Numerical Solution to Schrodinger's Equation for a One-Dimensional Finite Potential Well

Christian B. Molina

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Abstract

Schrodinger's Equation and the potential well is used to introduce the quantum mechanics of a particle of mass confined by a surrounding constant potential. Detecting the position of a particle of mass in such a system begins to deviate from the expectations of classical physics, rather the particle has the probability of occupying certain positions in space based on its energy level. The probability of the particle's position exhibits the behavior of a harmonic oscillator, in which there is nodes defined throughout space. This allows us to describe a wave function for the particle's probability density in a one-dimensional infinite and finite potential well using Schrodinger's Equation. Solving the wave function for the infinite potential well can be done analytically, while the solution for the finite potential results in a transcendental equation, which can be solved numerically.

In this report, the wave function of the probability density for an proton in an finite potential well of depth $U_0 = 10MeV$ and width $L = 7fm$ will be solved numerically using outlined algorithms.

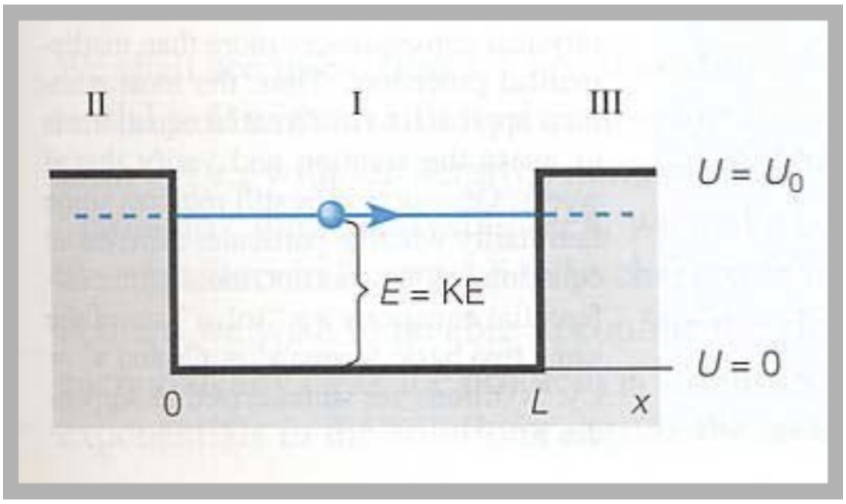

Figure 1: Finite potential well

1 Introduction

1.1 Time-Dependent Schrodinger's Equation

Schrodinger's Equation for a Free-Particle Wave Function is defined as :

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t} \tag{1}$$

The wave function can be defined as:

$$\Psi(x,t) = \psi(x)\phi(t) \tag{2}$$

For the Particle in a Box, we are limiting the wave function to only one spatial dimension of the equation and will be defined as:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x) \tag{3}$$

Where U(x) is the potential energy and E is the energy of the system.

1.2 The Infinite Potential Well

The Particle in a Box for a Infinite Potential is a system in which the particle is confined to a rectangular region surrounded by infinite potential. The parameters of the potential are as follows:

$$U = \begin{cases} 0 & 0 < x < L \\ \infty & 0 > x, L < x \end{cases} \tag{4}$$

In this report, Region I will be defined as $0 < x < L$, and regions II and III will be defined as $x < 0$ and $x > L$ respectively.

Inside Region I, the particle is able to act as a free particle, while in regions II and III the particle is not defined. The spatial probability wave function can then be defined as:

$$\psi(x) = \begin{cases} A\sin(kx) + B\cos(kx) & 0 < x < L \\ 0 & x < 0, x > L \end{cases} \tag{5}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \tag{6}$$

The coefficients A and B are determined by considering the boundary conditions of $x = 0$ and $x = L$

Consider the continuity of $\psi(x)$ at x=0

$$\psi_{II(0)} = \psi_{I(0)}$$
$$0 = A\sin(k(0)) + B\cos(k(0))$$
$$B = 0$$

The second boundary condition:$\psi(x)$ continuous at $x = L$ yields:

$$\psi_{I(L)} = \psi_{III(L)}$$
$$0 = A\sin(kL)$$
$$kL = n\pi$$

From the last condition, it is found that:

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

Therefore:

$$\psi_n(x) = A\sin\frac{n\pi}{L}x \qquad 0 < x < L \tag{7}$$
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{8}$$

Equation (8) indicates that certain quantized energy levels are allowed.
Using the condition of Normalization, the coefficient A can then be solved for:

$$\int_{allspace} |\psi(x,t)|^2\,dx = \int_{-\infty}^{\infty} |\psi(x)|^2\,dx = \int_0^L A\sin\frac{n\pi}{L}x^{\,2}\,dx = 1 \tag{9}$$

$$\begin{aligned} A^2\frac{L}{2} &= 1 \\ A &= \sqrt{\frac{2}{L}} \end{aligned} \tag{10}$$

1.3 The Finite Potential Well

The Finite Potential well is an extension of the Infinite Potential well. Rather than having an infinite potential, the potential is finite. The Finite Potential well presents an additional layer of quantum behavior: the particle now has the probability of being measured outside the box - this is considered quantum tunneling.

The procedure for finding the energies and wave function of the Finite Potential well is similar to the Infinite Potential well, but instead with a finite potential barrier:

$$U = \begin{cases} U_0 & x < 0 \\ 0 & 0 \le x \le L \\ U_0 & L < x \end{cases} \tag{11}$$

In this system, the particle is bound to $U = 0$ within the well, Region I. However, at $x < 0$ and $x > L$ - regions II and III respectively - the energy of the particle is bound to $U = U_0$. Therefore all regions must be considered when defining the wave function.

The conditions satisfying the time-independent Schrodinger Equation - equation (3) - and normalization is the same. However, the wave function defined in regions II and III are nonzero. The wave function $\psi(x)$ is defined as:

$$\psi(x) = \begin{cases} Ce^{\alpha x} & x < 0 \\ A\sin(kx) + B\cos(kx) & 0 < x < L \\ Ge^{-\alpha x} & x > L \end{cases} \tag{12}$$

Similar to the Infinite potential well, the boundary conditions can be used to find relations between coefficients and constants:

Continuity of $\psi(x)$ at $x = 0$

$$\psi_{II(0)} = \psi_{I(0)}$$
$$Ce^{\alpha 0} = A\sin(k(0)) + B\cos(k(0))$$
$$C = B$$

$\psi'(x)$ at $x = 0$

$$\psi'_{II(0)} = \psi'_{I(0)}$$
$$\alpha Ce^{\alpha 0} = kA\cos(k(0)) - kB\sin(k(0))$$
$$\alpha C = kA$$

$\psi(x)$ at $x = L$

$$\psi_{III(L)} = \psi_{III(L)}$$
$$A\sin(kL) + B\cos(kL) = Ge^{-\alpha L}$$

$\psi'(x)$ continuous at $x = L$

$$\psi'_{I(L)} = \psi'_{III(L)}$$
$$kA\cos(kL) - kB\sin(kL) = -kGe^{-\alpha L}$$

Utilizing the results of the last two boundary conditions, we find the transcendental equation:

$$2\cot kL = \frac{k}{\alpha} - \frac{\alpha}{k} \tag{13}$$

Equation (13) cannot be solved analytically. In this report, the transcendental equation will be solved numerically.

2 Methods

2.1 Algorithm: Finding Roots of Transcendental Equation

In order to solve the wave function for the Finite Potential well, the roots of the transcendental equation - equation (13) - must be found.

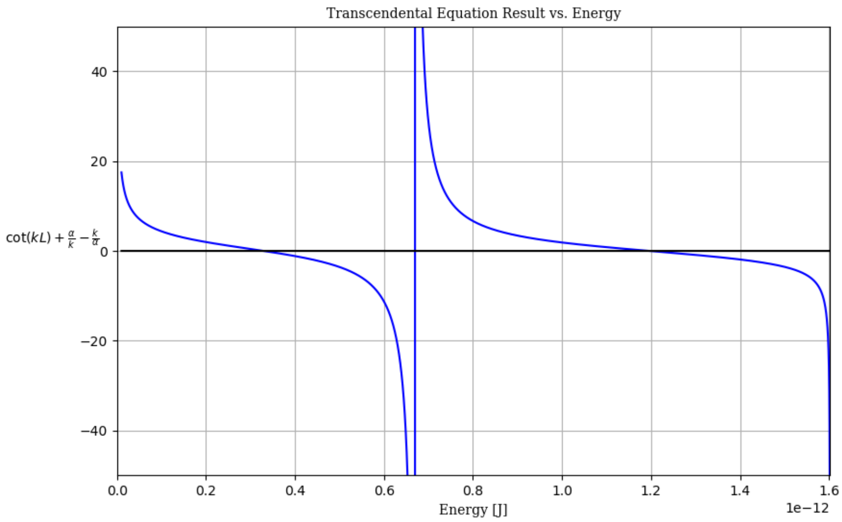

Figure 2: Roots of transcendental equation are wherever function crosses x-axis

The following algorithm requires that a range of values for E are calculated for the transcendental equation. Equation (13) can be directly translated into code and thus generate results stored in an array. In this algorithm such an array will be defined as *trans_results*

Algorithm 1: Find roots of transcendental equation

Result: Return energy roots of transcendental equation
E_values: array of energy values ranging from zero to U_0;
approxZero= $1e - 14$;
trans_results: array of results from equation (13);
while $n = 0 <$ *length of trans_results*, $n++$ **do**
  if *trans_results[n]* $< approxZero/U_0$ ***and*** *trans_result* ≥ 0 **then**
    append E_values into roots array;
  end
end

Algorithm 1 indexes through the calculated results of equation (13) and determines which value is closest to zero. There are no actual results that are exactly zero, and this is because of the increment steps between values for the original range of E values. Instead this algorithm selects indices that contain non-negative values less then an approximated zero. Once these indices are selected, the corresponding E-value is saved to an array called roots.

As a disclaimer, there will be various values of the transcendental equation results that are less than the approximated zero. In this algorithm, it allows all values that fulfill the if-condition be stored into the root array, but it recommended that the user selects the first and last values of the roots array. There are only two roots, as seen in figure 2, and the first and last elements of the roots array will correspond to those roots but with insignificant variation.

Once the roots are found, they can be utilized to find constants A,B,C and G. by plugging in the roots for each boundary condition and isolating certain constants

3 Discussion

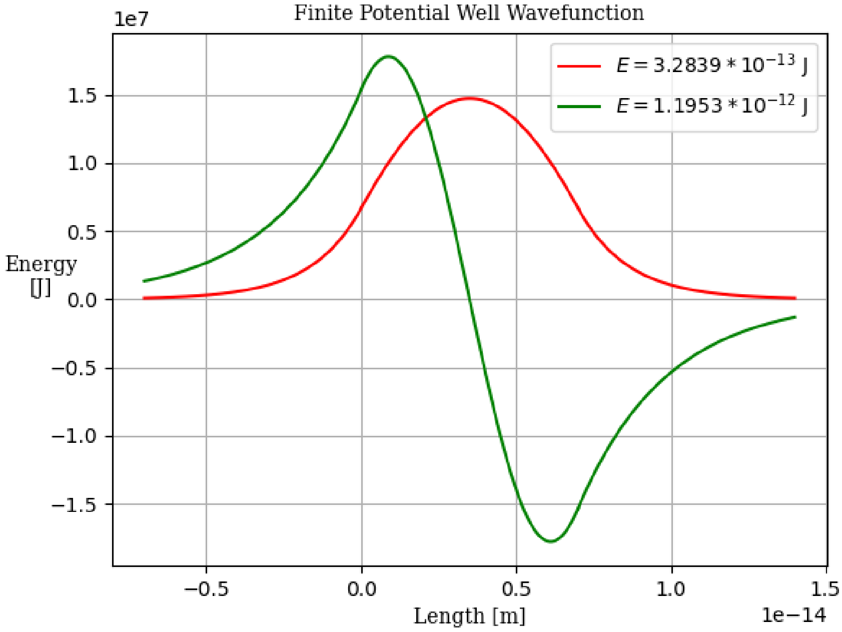

Figure 3: Wave function for Energy values: **3.289e-13 J** and **1.195e-12 J**

Figure 3 displays the wave functions of the Finite Potential well for energy values 3.2839×10^{-13} J and 1.1953×10^{-12} J. In figure 3, there is continuity in from region I to both region II and III. This corresponds to the normalization of the Finite potential well:

$$\int_{allspace} |\psi(x,t)|^2\, dx = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx =$$
$$\int_{-\infty}^{0} (Ce^{\alpha x})^2\, dx + \int_{0}^{L} (A\sin(kx) + B\cos(kx))^2\, dx + \int_{L}^{\infty} (Ge^{-\alpha x})^2\, dx = 1$$

4 Conclusion

With the infinite well, it is expected to have various wave functions based on the energy states. This analysis of the finite potential well shows that the wave function is limited to only certain energy states because of the finite value of the potential well. This also shows the behavior of quantum tunnelling.