Shröedinger's Equation for a Particle Confined to a Finite 1-D Potential Well

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Abstract

In this experiment, we examine the wave like behavior for a proton in a rectangular potential well of width $L = 7 * 10^{-15}$ [m] and depth $U_0 = 10$ [MeV]. The premise of this project is to obtain the allowed energies and wavefunction for this particle by solving the Shröedinger Equation. The Shröedinger equation for a Finite Well is a transcendental function, thus cannot be solved analytically. The ground state energy for a proton under these conditions, as well as all wave functions were found by determining the roots of the transcendental function (i.e. where the transcendental output versus energy was 0) and confirmed graphically. These energies were then utilized to determine the coefficients of the wave function. Comparing the Finite Well wave functions to the Infinite Well wave functions of the same conditions, we find that their behavior is in agreement with what is expected: quantum tunneling occurs for energies of the finite well in previously forbidden regions, where as no energies are allowed beyond the well for the infinite well.

1 Introduction

1.1 Infinite Potential Well

A particle confined to a potential well exhibits wave like properties. It is a common example that showcases the quantum properties of matter. Inside the region $0 < x < L$ the wave function must be a solution of the time-independent, non-relativistic Schröedinger equation:

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

The finite well is depicted as follows:

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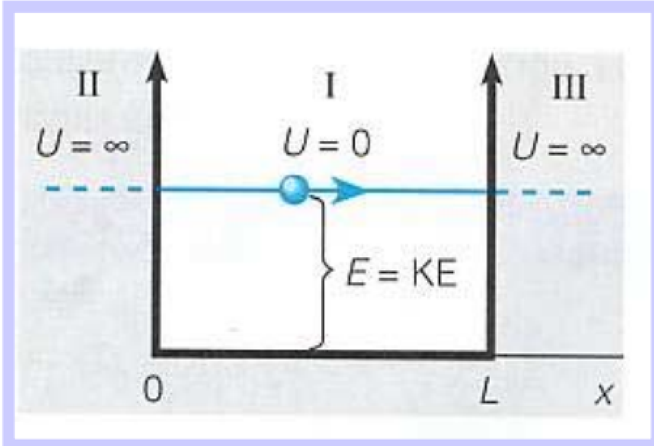

Figure 1: The Infinite Potential Well of length L and potential U_0

We will describe the region $0 < x < L$ as Region I, and the regions $x < 0$ & $x > L$ as Region II and Region III respectively.

Beginning with the simpler case of a bound particle, the infinite well proves to be a good starting place. The particle is bound to the potential well with at $U = 0$ within the range $x = 0$ and $x = L$. Outside of this region, there is infinite potential, thus a wave function outside of the potential well must be 0. Since the potential has infinite potential everywhere outside the well, the primary region of interest is $0 < x < L$.

$$U = \begin{cases} 0 & 0 < x < L \\ \infty & 0 > x, L < x \end{cases} \tag{2}$$

However, $U(x) = 0$, thus the following function defines the wave function of Infinite Potential Well:

$$\psi(x) = \begin{cases} A\sin(\kappa * x) + B\cos(\kappa * x) & 0 < x < L \\ 0 & 0 > x, L < x \end{cases} \tag{3}$$

where

$$\kappa = \sqrt{\frac{2mE}{\hbar^2}} \tag{4}$$

The coefficients A and B are determined by utilizing the boundary conditions at $x = 0$ and $x = L$. We consider the first: $\psi(x)$ continuous at $x = 0$

$$\psi_{II(0)} = \psi_{I(0)} 0 = A\sin(k * 0) + B\cos(k * 0) B = 0 \tag{5}$$

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

$$\psi_{I(L)} = \psi_{III(L)} 0 = A\sin(k * L) k * L = n * \pi \tag{6}$$

From this last condition we find:

$$\begin{gathered} \sqrt{\frac{2mE}{\hbar^2}} L = n\pi \\ E = \frac{n^2\pi^2\hbar^2}{2mL^2} \end{gathered} \tag{7}$$

And finally:

$$\begin{cases}\psi_n(x) = A\sin\frac{n\pi}{L}x & 0 < x < L\end{cases} \tag{8}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{9}$$

What (9) tells us is that only certain energies are allowed, and that these values are discrete. Utilizing the last condition of normalization of the wave function, we solve for constant A:

$$\int_{allspace} |\psi(x,t)|^2\,dx = \int_{-\infty}^{\infty} |\psi(x)|^2\,dx = \int_0^L A\sin\frac{n\pi}{L}x^2\,dx = 1 \tag{10}$$

$$\begin{aligned} A^2\frac{L}{2} &= 1 \\ A &= \sqrt{\frac{2}{L}} \end{aligned} \tag{11}$$

1.2 Finite Potential Well

The procedure for finding the energies and wave function of the Finite Potential Well is similar to the Infinite, however a bit more involved as regions II and III are no longer infinite, however the conditions of satisfying the time-indepdent, non-relativistic Shröedinger Equation (1) and normalization remains the same. The Finite Potential Well is depicted by the following diagram:

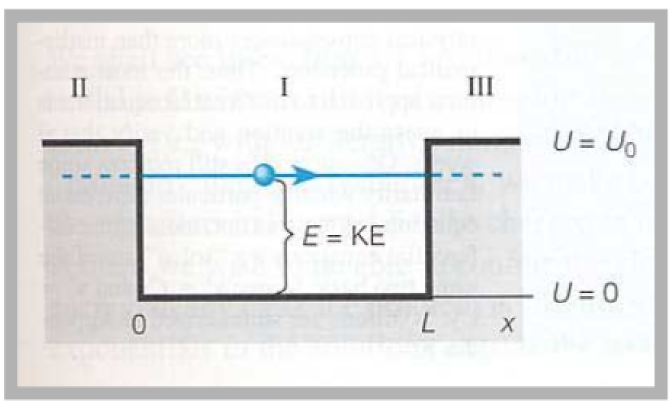

Figure 2: The Finite Potential Well of length L and potential U_0

In this scenario, the particle is bound to $U = 0$ within the well. However, at $x < 0$ and $x > L$, the energy of the particle is bound to $U = U_0$. All regions must be examined.

$$U = \begin{cases} U_0 & x < 0 \\ 0 & 0 \le x \le L \\ U_0 & L < x \end{cases} \tag{12}$$

For the finite potential well, $\psi(x)$ is described by

$$\psi(x) = \begin{cases} Ce^{\alpha * x} & x < L \\ A\sin(\kappa * x) + B\cos(\kappa * x) & 0 < x < L \\ Ge^{-\alpha * x} & L < x \end{cases} \tag{13}$$

Similarly to the infinite potential well, we utilize the boundary conditions to find the relations between the constants. We first look at the boundary condition:

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

$$\psi_{II(0)} = \psi_{I(0)} Ce^{\alpha 0} = A\sin(k*0) + B\cos(k*0)C = B \tag{14}$$

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

$$\psi'_{II(0)} = \psi'_{I(0)} \alpha Ce^{\alpha 0} = \kappa A\cos(k*0) - \kappa B\sin(k*0)\alpha C = \kappa A \tag{15}$$

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

$$\psi_{I(L)} = \psi_{III(L)} A\sin(k*L) + B\cos(k*L) = Ge^{-\alpha L} \tag{16}$$

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

$$\psi'_{I(L)} = \psi'_{III(L)} \kappa A\cos(k*L) - \kappa B\sin(k*L) = -\alpha Ge^{-\alpha L} \tag{17}$$

Utilizing (16) and (17), we find the transcendental equation:

$$2\cot\kappa L = \frac{\kappa}{\alpha} - \frac{\alpha}{\kappa} \tag{18}$$

The purpose of this lab is to utilize this equation to first determine the energy levels of the proton, and then the total wave equation with all constants solved.

1.3 Procedure

The goal is to solve for the energies and wave function of a proton confined to a finite well of $L = 7*10^{-15}m$ and $U_0 = 10*10^6 MeV$. The following is the pseudocode detailing this process.

1. Find the roots of the transcendental function (18)

    2. Plot the transcendental equation as a function of energy to confirm roots

    3. Determine the α and κ values for each energy

    4. Check how closely the energy value obtained satisfies the transcendental function (how close to 0?)

5. Find constants A,B,C,G

    6. Isolate constant C for all equations of $\psi(x)$, then utilizing the fact that the normalization for all space must equal 1, (10), solve for C.

    7. Utilize the relationships from the boundary conditions to solve for all other variables

    8. Determine constants A,B,C,G for all energy levels

9. Plot the Finite Well Wave Function for all corresponding energies

10. Compare the Finite Well to the Infinite Well for the same conditions

    11. Plot the infinite well independently, then make a graphical comparison to the finite well

1.4 Discussion

For a proton confined to a finite potential well of length $L = 7 * 10^{-15}m$ and potential $U_0 = 10 * 10^6 eV$, two energy levels were found. To test the validity of these energies, a range of energies between $U_0 * 10^{-3}$ to $U_0 * 10^3$ were plotted against the transcendental output, and it was found that the energies were indeed correct. The following figure acts as confirmation.

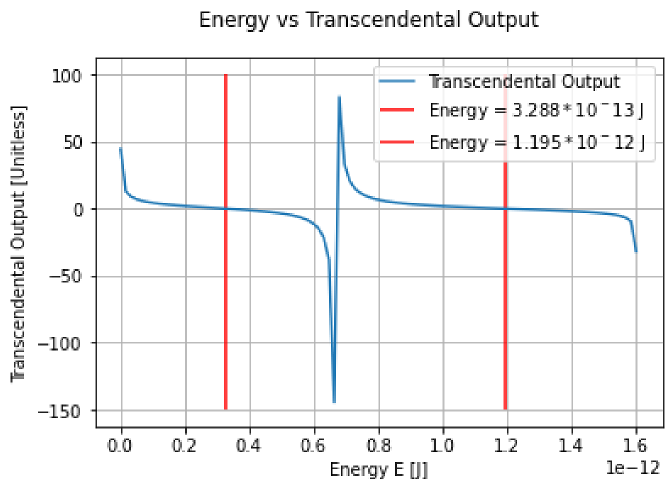

Figure 3: Determining The Validity of Calculated Energy Values Utilizing the Transcendental Function

Solving for the constants, the wave function was then plotted for each of the energies found within the following figure:

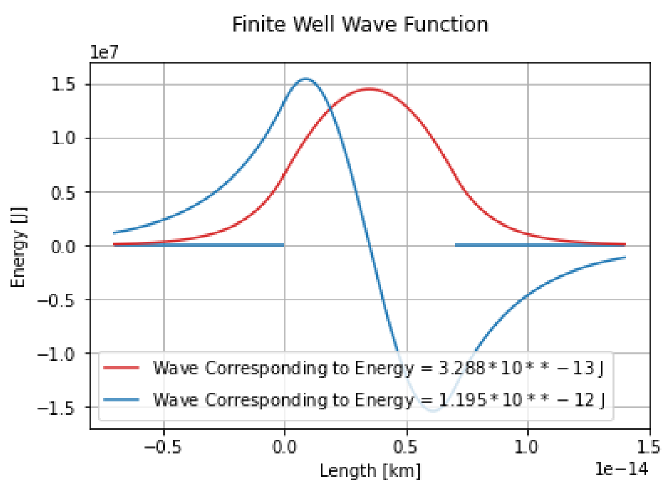

Figure 4: The Wave Function for a Proton Confined to a Finite Well of length $L = 7*10^{-15}m$ and potential $U_0 = 10 * 10^6 eV$

The finite and infinite well are simplified cases of the Shröedinger Equation. Comparison of the two allows us to determine the the wave like properties of particles to predict their distribution and behavior. The following is a plot of the discrete energy levels of the infinite well with the same well width.

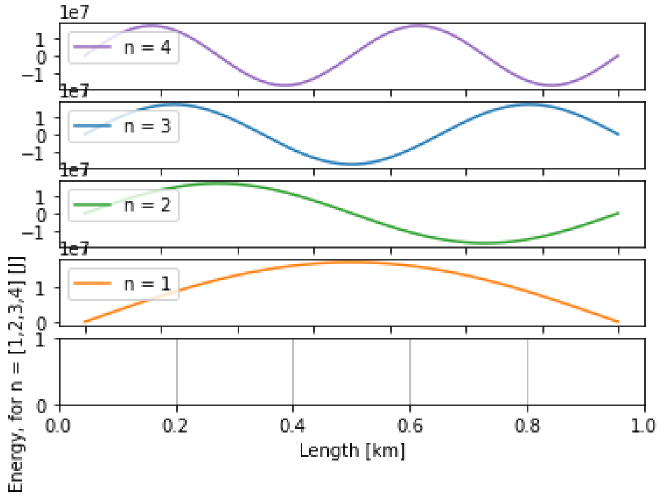

Figure 5: Wave Functions for Discrete Energy Levels n = 1, 2, 3, 4 for the Infinite Potential Well of length $L = 7 * 10^{-15} m$ and potential $U_0 = 10 * 10^6 eV$

We see the effects of quantum tunneling when comparing the two, as depicted in the following graph. Ordinarily forbidden energy levels of the infinite well are possible within the finite well, however outside of the well, $U \neq U_0$ instantly outside of $0 < x < L$.

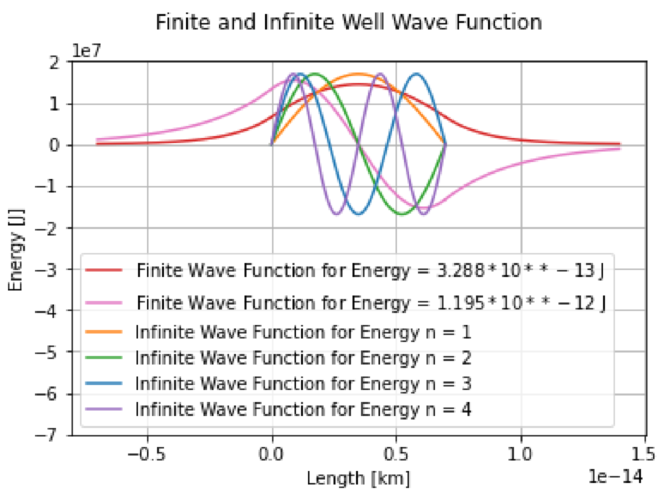

Figure 6: The Finite Potential Well and Infinite Well of length L and potential U_0

Table 1: Summary of Constant Values for Energy Levels Found

	$3.288 * 10^{-13}$ **[J]**	$1.195 * 10^{-12}$ [J]
Constant A	12889007.937...	7750261.017...
Constant B	6549913.847...	13288302.355...
Constant C	6549913.847...	13288302.355...
Constant G	498254445.367...	-153713495.246...

2 Conclusion

Comparing the finite well and infinite well, we expect that the finite well will have less possible energy states as there is a limit to the number of states the photo is able to occupy. Also, the corresponding energies for the finite well are less than that of the infinite well for the same well width L. This is also expected as the proton in the infinite well is not as strictly bound as in the finite well. Overall, this project is in agreement and supports what is known of particles confined to infinite and finite wells.