Solving the Particle in a Box Problem Using Newton's Method

Nicholas Chu, Fletch Hoppe, David Llewellyn Smith, Emily Murrell

July 22, 2024

1 Introduction

The finite square well is a problem in quantum mechanics. It considers a particle inside a so-called "box" in which the "walls" on either side are the potential energy of the system. That means:

$$V(x) = \begin{cases} -V_0, & -a \leq x \leq a, \\ 0, & a \leq |x|, \end{cases} \tag{1}$$

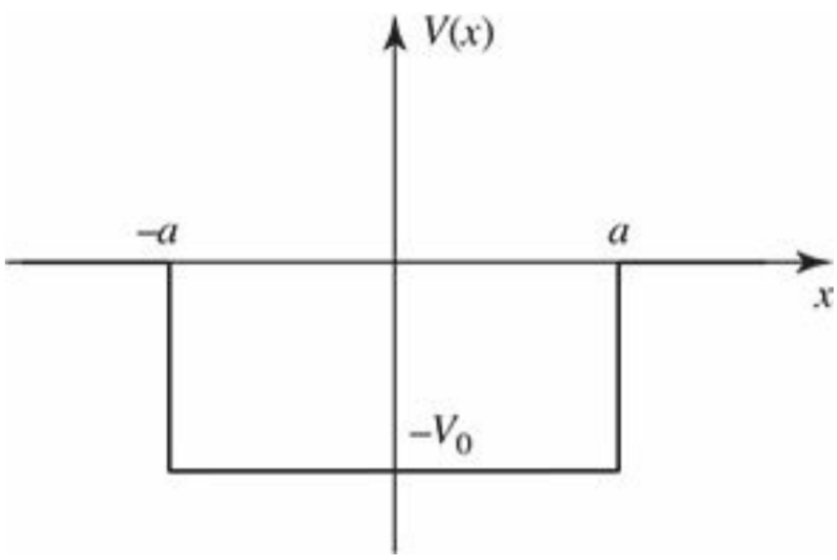

Figure 1: Potential energy in the finite square well. Taken from Griffiths.

Solving the problem using Schrödinger's equation returns a transcendental equation - one that doesn't have a closed-form solution. However, using Newton's Method, we can approximate the solutions and find the energy levels of a particle in a finite square well.

2 Methodology

2.1 Solving Schrodinger's Equation

This potential, combined with the Schrodinger Equation, reduces to a symmetric piecewise differential equation. Namely, while within the potential well ($-a \leq x \leq a$),

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = (E + V_0)\Psi \tag{2}$$

where E is the total energy of the particle, a constant for a particular solution. Outside the well ($|x| \geq a$), the Schrodinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi \tag{3}$$

These differential equations have the same form as the simple harmonic oscillator. That means we can guess similar solutions. We assume the particle is bound, so there is a high probability of it being within the well. Using the fact that the potential is symmetric we guess that the solution within the well ($-a \leq x \leq a$) is

$$\Psi(x) = Bcos(lx),\ with\ l = \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{4}$$

Using the fact the particle is bound its wavefunction should decay as $|x| \to \infty$. For the area to the left of the well ($x < -a$) we guess and verify the solution:

$$\Psi(x) = Ae^{-\kappa x},\ with\ \kappa = \frac{\sqrt{-2mE}}{\hbar} \tag{5}$$

A and B may be found by imposing a normalization condition on the wavefunction ($\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$), but the most important remaining calculation is the energy. This will determine κ and l and tell us the most about the particle. This may be accomplished through the use of boundary conditions at the edges of the well. The wavefunction must be continuous at the boundaries ($\lim_{x\to -a^-} \Psi(x) = \lim_{x\to -a^+} \Psi(x)$). Further, its derivative must be continuous as it represents the flow of probability of the particle. Probability flow into the well from the left must be the same as negative probability flow out from the right, yielding the additional condition that $\lim_{x\to -a^-} \frac{d\Psi(x)}{dx} = \lim_{x\to -a^+} \frac{d\Psi(x)}{dx}$.

Out of convenience, we'll use $z = la$ and $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$. Using this shorthand and imposing these conditions on the earlier piecewise wavefunction and doing a bit of algebra yields two equations, for the even and odd solutions respectively:

$$tan(z) = \sqrt{(z_0/z)^2 - 1}, \tag{6}$$

$$cot(z) = -\sqrt{(z_0/z)^2 - 1} \tag{7}$$

These are transcendental equations, so they cannot be solved analytically. However, a numerical method still works, so we will apply Newton's Method to the functions

$$f(z) = tan(z) - \sqrt{((z_0/z)^2 - 1}, \tag{8}$$

$$g(z) = cot(z) + \sqrt{(z_0/z)^2 - 1}, \tag{9}$$

$$f'(z) = sec^2(z) + \frac{z_0^2}{z^2\sqrt{z_0^2 - z^2}}, \tag{10}$$

$$g'(z) = -csc^2(z) - \frac{z_0^2}{z^2\sqrt{z_0^2 - z^2}} \tag{11}$$

2.2 Newton's Method

To solve 6 and 7 we will use Newton's method. Before we use Newton's Method, we will briefly explain what it is. Newton's Method is a numerical root finding algorithm. It works by approximating a function as a line by using the function's value and the value of its derivative at a point. The root of this linear approximation of the function is then found and the process is repeated with that new x value. Succinctly, Newton's Method is an iterative function of the following form, where x_{n+1} is the next guess for the root after x_n:

$$x_{n+1} = x_n - \frac{f(x)}{f'(x)} \tag{12}$$

The theory for Newton's Method likewise states that for our transcendental equation, Newton's Method will converge quadratically, roughly doubling the number of accurate digits with each iteration. This is because the root we are searching for has multiplicity 1. Further, because we are working with sinusoidal functions, we may have multiple solutions to the transcendental equation. This corresponds to different Quantum level solutions to the same potential.

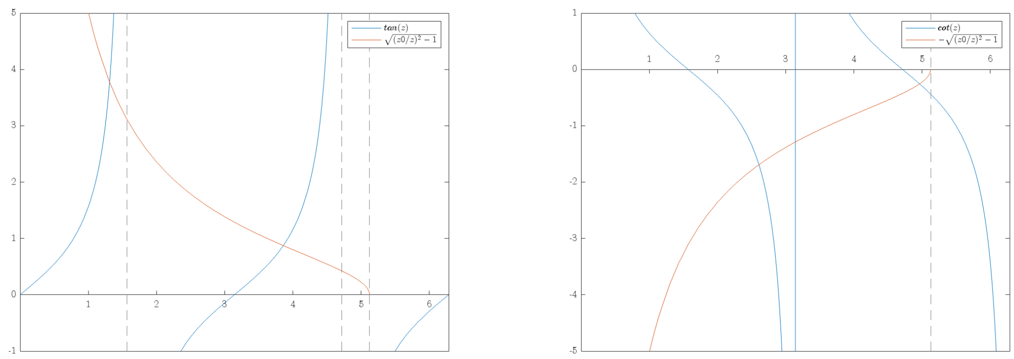

Figure 2: Graphical solutions to energy levels for $a = 1nm$, $m = 9.11 * 10^{-31}kg$, $V_0 = 1eV$

2.3 Pseudocode

The pseudocode for the program used is as follows. $f(x)$ is the function whose root is to be found, $f'(x)$ is its derivative, x_0 is an initial guess, and $Threshold$ is the value of $f(x)$ for which our guess of a root is sufficiently good that it can be returned.

Algorithm 1 Newton's Method

Require: $f(x), f'(x), x_0, Threshold$
  $n \leftarrow 0$
  while $|f(x_n)| > Threshold$ **do**
    $x_{n+1} = x_n - f(x_n)/f'(x_n)$
    $n \leftarrow n + 1$
  end while
  return x_n

2.4 Solving the Energies

Because of the sinusoidal part of our function $f(z)$, we anticipate the existence of multiple solutions. To account for these, we used Newton's method multiple times, alternating between the even and odd solutions, with initial guesses spaced by $\frac{\pi}{2}$. We considered the case of an electron in a well with width $2nm$ and potential $1ev$. Using these values, we finally applied Newton's Method to our transcendental equations 8 and 9, and using different initial guesses to find the different roots, we arrived at the following values:

z Initial Guess	z	f(z)	E (Joule)	κ (m^{-1})	l (m^{-1})
0.01	1.3119	$2.5609 * 10^{-11}$	$-1.4971 * 10^{-19}$	$4.9523 * 10^9$	$1.3119 * 10^9$
$\pi/2 + 0.01$	2.6076	$-1.5417 * 10^{-9}$	$-1.187 * 10^{-19}$	$4.4097 * 10^9$	$2.6075 * 10^9$
$\pi + 0.01$	3.8593	$3.0259 * 10^{-11}$	$-6.92992 * 10^{-20}$	$3.36936 * 10^9$	$3.8593 * 10^9$
$3\pi/2 + 0.01$	4.9630	$-3.2752 * 10^{-15}$	$-9.8551 * 10^{-21}$	$1.2706 * 10^9$	$4.9628 * 10^9$

3 Discussion

In this experiment, with an initial guess of 0.01, we found that Newton's Method approximated the root of $f(z)$ to be 1.3119 after rounding to 4 decimal places. We also used initial guesses of $\frac{\pi}{2}$ + 0.01, π + 0.01, and $\frac{3\pi}{2}$ + 0.01, alternating between even and odd solutions to account for all of the solutions, getting 2.6076, 3.8593, and 4.9630 respectively for our approximations of the roots. However, these values of z are dimensionless and uninterpretable; what is of most importance is the value of E that we get from z. We see from our results that there is only a certain amount of possible energy levels even when offsetting our initial guesses: this is because the right side of 7 is the equation of a circle and undefined for large enough z. This provides a physical limit on the energy of the particle in the system.

4 Conclusion

Newton's method proved to be an effective way to find energy values for the particle in a box problem. As said above, even though this method gave values of z that are unable to be interpreted on their own, it did allow us to get close approximations of the energy levels of the particle (to 10^{-5} because of our threshold). These values are (in Joules) $-1.4971*10^{-19}$, $1.187*10^{-19}$, $6.92992*10^{-20}$, and $-9.8551 * 10^{-21}$. Using Newton's method allowed us to find close approximations of values that would be impossible to solve for exactly otherwise.

5 References

[1] Griffiths, D. J., & Schroeter, D. F. (2018). Introduction to Quantum Mechanics (3rd ed.). Cambridge: Cambridge University Press.
[2] Burden, R.L., & Faires, J.D. (2011) Numerical Analysis (10th ed.). Boston: Cengage Learning.