PHY 520 Quantum Mechanics Infinite and Finite Square Well TISE Solutions Report

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# Abstract

In this report, I present my portion of Group 4’s work on solutions and simulations to various Time Independent Schrӧdinger’s Equation potentials (TISE): the Infinite and Finite Square Well Potential. I present the method to obtaining solutions for only the bound states of each potential. I end by presenting the simulation applet, which was built in Mathematica to investigate how the solution changes with varying parameters, such as well depth, energy, and well width.

# Preliminary

In the following documentation, we will focus on solving for eigenfunctions of different potentials: the Infinite and Finite Square Wells. We begin with the TISE:

$\frac{-ℏ^{2}}{2m}\*\frac{d^{2}Ψ(x)}{dx^{2}}+V\left(x\right)Ψ\left(x\right)=E\_{n}Ψ\_{n}\left(x\right)$

From Griffith’s chapter two, we must recall the boundary conditions to be evaluated when finding solutions to the TISE:

1. $Ψ\left(x\right) $is continuous everywhere.
2. $\frac{dΨ}{dx}$ is continuous everywhere except where the potential may be infinite

The above conditions, as well as normalizing the wave function, will help us find various coefficients in the solutions for each of our wells. This will help us “stitch together” solutions across boundaries of the potentials.

The strategy to solving this equation is the following:

* First write down the TISE with the specific potential of interest$ V \left(x\right)$.
* Apply the above boundary conditions to find the most general solution.
* Normalize the wave function in order to find the coefficients in the solution.
* Write out the total solution with all solved-for coefficients.

We now begin with the specific case: What if$ V\left(x\right)=\left\{\begin{array}{c}0,\\\infty ,\end{array} \genfrac{}{}{0pt}{}{0\leq x\leq a}{otherwise}\right.$?

# The Infinite Square Well Potential

The infinite square well is the most straight forward non-zero potential we will cover. This square well is given by the following function:

$$V\left(x\right)=\left\{\begin{array}{c}0,\\\infty ,\end{array} \genfrac{}{}{0pt}{}{0\leq x\leq a}{otherwise}\right.$$

This function is defined in the opening of the infinite well applet. Particles under the influence of this potential are free between $x=0$ and$ x=a, $or whatever we define the bounds to be. However, outside that region$ Ψ\left(x\right)=0$, meaning that the particle is completely excluded outside the well.

 To find the eigenfunctions or solutions for this potential, we start by evaluating the Time Independent Schӧdinger Equation:

$$\frac{-ℏ^{2}}{2m}\*\frac{d^{2}Ψ(x)}{dx^{2}}+V\left(x\right)Ψ\left(x\right)=E\_{n}Ψ\_{n}\left(x\right)$$

Inside the well our potential is equal to zero. This leaves only the first term of the Hamiltonian to be evaluated, turning it into a simple differential equation whose solution is simply:

$Ψ\left(x\right)=Asin\left(kx\right)+Bcos(kx)$ where $k=\frac{\sqrt{2mE\_{n}} }{ℏ}$

Constants A and B are fixed by the potential’s boundary conditions; where $Ψ\left(x\right)$ and $\frac{dΨ}{dx}$ are continuous. Once boundary conditions are evaluated we find that our wave function only contains one term.

$Ψ\_{n}\left(x\right)=\sqrt{\frac{2}{a}} sin⁡(\frac{nπ}{a}x)$ where $k\_{n}=\frac{nπ}{a}$

 Now that we have determined k for various n values we can determine the energy spectrum of the potential well.

$$E\_{n}=\frac{ℏ^{2}n^{2}π^{2}}{2ma^{2}}$$

The above eigenfunctions hold four main properties. First they are alternately even and odd with the respect to the center of the well. This property has been accounted for in the applet and will be described latter in the document. Second: as you go up in energy, every other state has one more node than the one before. The last two properties held by the solutions are that they are complete and a set of mutually orthogonal eigenfunctions.

# Mathematica Simulation: Infinite Square Well

With Mathematica, we can simulate the above results to learn more about the system. The program I wrote is basically a plot of the solutions for various energy levels. In order to account for the alternating even and odd solutions, a shift was added to the code. The program allows you to adjust $a$ and$ b$, which control the width of the infinite well, and the energy level of the wave. Mass and Planck’s constant were define as one for this simulation. Figure 1 show’s a typical plot from the applet.



Figure 1: Bound states of the infinite square well potential. Note that blue represents the wave, orange is the potential well, and green is the energy level of the wave.

# The Finite Square Well

The finite square well is the last potential we will cover. This square well is given by the following function:

$$V\left(x\right)=\left\{\begin{array}{c}-V\_{0},\\0,\end{array} \genfrac{}{}{0pt}{}{-a\leq x\leq a}{\left|x\right|>a}\right.$$

This function is defined in the opening of the finite well applet. Particles under the influence of this potential are subject to bound and scattering states. For simplicity we will only focus on the bound states for this applet. This implies we are only dealing with negative values for energy$ (E<0)$. Let’s first evaluate the TISE in the first region, where$ x<-a$.

In this first region the potential is zero:

$$\frac{-ℏ}{2m}\*\frac{d^{2}Ψ(x)}{dx^{2}}=E\_{n}Ψ\_{n}\left(x\right)$$

$Ψ\left(x\right)=Be^{Κx}$ where $Κ=\frac{\sqrt{-2mE}}{ℏ}$

Our second term $Ae^{-Κx}$ blows up, as Griffith’s says, as x approaches negative infinity. Now we will evaluate the TISE where $-a<x<a$:

$$\frac{-ℏ}{2m}\*\frac{d^{2}Ψ\left(x\right)}{dx^{2}}-V\_{0}Ψ(x)=E\_{n}Ψ\_{n}\left(x\right)$$

$Ψ\left(x\right)=Csin\left(lx\right)+Dcos(lx)$ where $l=\frac{\sqrt{2m(E+V\_{0})} }{ℏ}$

By Symmetry the solutions to the region where $x>a $are as follows:

$Ψ\left(x\right)=Fe^{-Κx}$ where $Κ=\frac{\sqrt{-2mE}}{ℏ}$

 The next step is to evaluate the boundary conditions, as described in the Preliminaries section. We find in doing so, that B=F for even solutions and B=-G for odd solutions, where B, C, D, F, and G are constants.

$Ψ\_{even}\left(x\right)=\left\{\begin{matrix}Fe^{-Κx}&x>a\\Dcos(lx)&-a<x<a\\Fe^{Κx}&x>-a\end{matrix}\right.$ $Ψ\_{odd}\left(x\right)=\left\{\begin{matrix}Ge^{-Κx}&x>a\\Csin(lx)&-a<x<a\\-Ge^{Κx}&x>-a\end{matrix}\right.$

The above coefficients can be found by normalizing the odd and even wave functions for the bound states. They were defined in the opening of the finite well applet. To solve for the allowed energies we will impose boundaries conditions. We find that:

$$Κ=ltan(la)$$

Since $Κ$ and l are both functions of E, we will solve for E by introducing the following variables:

$z=l\*a$ $z\_{0}=\frac{a}{ℏ}\sqrt{2mV\_{0}}$

From the formulas of $Κ$ and$ l$, it follows that

$$\tan(\left(z\right))=\sqrt{\left(\frac{z\_{0}}{z}\right)^{2}-1}$$

By solving for z in the above equation, and using$ z=l\*a, $we can solve for the allowed energies.

# 5 Mathematica Simulation: Finite Square Well

With Mathematica, we can simulate the above results to learn more about the system. The program I wrote is basically a plot of the odd and even solutions for various energy levels. Although we know that solutions alternate between even and odd functions, I plotted both separately to observe the boundary condition violations. The program allows you to adjust$ a$, which controls the width of the finite well, the energy level of the wave, and $V\_{0}$ the potential well depth. Mass and Planck’s constant were define as one for this simulation. Figure 2 show’s a typical plot from the applet.



Figure 2: Even and odd bound states of the finite square well potential. Note that blue represents the even solutions, orange is the odd solutions, yellow is the energy level, and green is the potential well.

As the energy bar is moved, we can observe boundary condition violations. This helps the user understand the transition from odd to even solutions, and why one or the other does not work for specific energy levels.