PHYS 240: Computational Physics Project
Numerical Solution to Quantum Tunneling

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May 20, 2017

1 Introduction

The goal of this project is to simulate the motion of a wave packet representing a quantum particle traveling through space which comes in contact with a potential step function. The equation of motion will come from the solution to the Schrodinger Equation and will be solved for numerically using an ODE step function solver. The transmission and reflection coefficients can be calculated and applied to the wave packet as it is split into a tunneled wave packet and a reflected wave packet. The time varying solution will then be plotted over space and viewable in movie format.

2 Model

The motion of a traveling quantum particle represented by a wave packet of energy E in free space can be described by the Schrodinger Equation.

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = (-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})\psi(x,t) = E\psi(x)$$

When the qauntum particle comes into contact with a potential barrier the Schrodinger equation changes to include the effects of the potential.

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

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

Here V(x) is the potential energy function and is given as

$$V(x) = \begin{cases} 0 & x \leq -a, x \geq +a \\ V_o & -a < x < +a \end{cases}$$

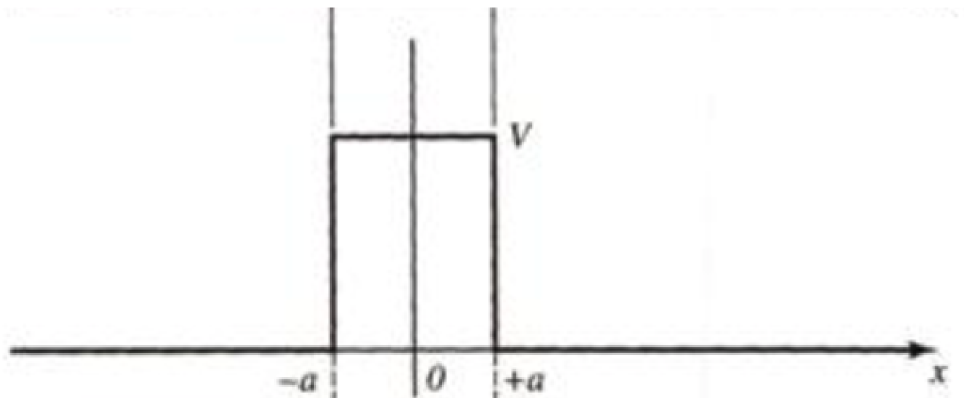

Figure 1: This figure shows a theoretical potential step function where V(x) = V from -a to +a and 0 everywhere else.[1].

Taking the added potential energy term into account, the soluiton, $\psi(x)$, will be piecewise [2].

$$\psi(x) = \begin{cases} Ae^{-i\sqrt{2mE/\hbar^2}x} + Be^{i\sqrt{2mE/\hbar^2}x} & x \leq -a \\ Ce^{-\sqrt{2m(V_o-E)/\hbar^2}x} & -a < x < +a \\ De^{-i\sqrt{2mE/\hbar^2}x} & x \geq +a \end{cases}$$

Where A,B, C and D are the amplitudes and are dependent on the physical conditions of the system. For this system the incident particle will be considered to enter from the left to the right, which is represented by the A term. The B term represents the wave as it is reflected off the potential step function and starts traveling back to the left. The third term only needs to consider right traveling motion represented by the D term, so there will be no left traveling term in the third equation.

What the second equation shows is that the particle will have a presence inside of the potential and as it travels through the potential the probability density diminishes. However, if the packet reaches the other end of the potential, at x = +a, before it decays to zero the packet will continue to travel out of the potential and back into free space where V(x)=0. The portion of the particle that did not pass through the potential barrier will be reflected back from the direction of incidence. This phenomenon is known as quantum tunneling and allows for a quantum particle to travel through the "classically forbidden" zones.

The core aspect to look for when studying quantum tunneling is the fraction of the particle that travels through the potential barrier and how much of it is reflected back. These quantities are known as the reflection (R) and transmission (T) coefficients. For the condition of $V_o > E$ they are defined as follows[5]

$$T = \frac{1}{1 + \frac{V_o^2 \sinh^2(2ka)}{4E(V_o - E)}}$$

where $k = \sqrt{2m(V_o - E)/\hbar^2}$ and R=1-T.

3 Numerical Method

To illustrate this behavior a program has been created that numerically solves the Schrodinger Equation and plots the solution. For a particle in free space its motion is described by this solution of the Schrodinger Equation. The evaluation is carried out using a method outlined by Garcia[3] for an implicit, iterative step function that solves the differential equation in the form of the Schrodinger Equation. Using numerical methods the equation is discretized in time and space.

$$\frac{\psi(x,t+\tau)-\psi(x,t)}{\tau}=\frac{i\hbar}{2m}\frac{\psi(x+\Delta x,t)+\psi(x-\Delta x,t)-2\psi(x,t)}{\Delta x}$$

The forward time step $\psi(x,t+\tau)$ can be solved for by isolating it on one side of the equality.

$$\psi(x,t+\tau)=\psi(x,t)+\frac{i\tau\hbar}{2m}\frac{\psi(x+\Delta x,t)+\psi(x-\Delta x,t)-2\psi(x,t)}{\Delta x}$$

This shows that by plugging in previous known values of $\psi(x,t)$ the future behavior can be modeled. This method is useful because it enables the use of computation in quickly solving and recording large systems of equations and is easy to extend to other differential equations of similar form.

By squaring $\psi(x,t)$, the probability density of the particle as a function of space and time is found. After the values for the particular time step has been evaluated and stored in a plot file the program loops through again with the updated values.

To kick start the numerical method the initial value for the iterative process is taken from the analytical solution to the wave packet function.

$$\psi(x,0)=\frac{1}{(\sqrt{2\pi\sigma_o})^{1/2}}e^{-\frac{(x-x_o)^2}{4\sigma_o^2}+ik_ox}$$

The known analytical solution in free space is in the form of a gaussian function[4], where σ_o is the initial width, x_o is the initial position and k_o is the initial wave packet energy. At t=0 the value of the solution can be used as the initial condition that is then carried through the numerical method calculations.

4 Implementation

The program is written in C++. It has variable parameters that can be input by the user of the physical system, such as the energy of the wave packet and the potential energy of the step function. These variable parameters affect the magnitudes of the transmission and reflection coefficients and alter how the potential barrier is plotted.

Through each iterative loop the evaluated ψ for the time step is stored in its own unique data file containing its spatial step and evaluated probability density. This data file can be used to plot the data using Gnuplot. By instructing Gnuplot to quickly display each plot one after the other the program will appear to show the wave packet moving in time.

The model is created using a spatial step value of $\Delta x = 0.33$ for 300 tics in space and a time step of $\tau = 5x10^{-4}$ for 200 time steps. All of which are changeable, however the parameters that were chosen were done so in order to preserve stability for the numerical method. Also, for simplicity the mass of the particle and $\hbar$ has been set to 1. This changes the magnitudes of the wave packets and their relation to the potential energy barrier, but not the overall behavior.

5 Results

The result of the program is a simulation of how the wave packet travels in free space and then is split into transmitted and reflected packets as it comes in contact with a potential barrier. The first image shows an incident particle of energy 0.35 approaching a barrier of energy 0.5. The next image is of the packet being split in two, with the transmitted packet continuing to travel to the right and the reflected packet moving left.

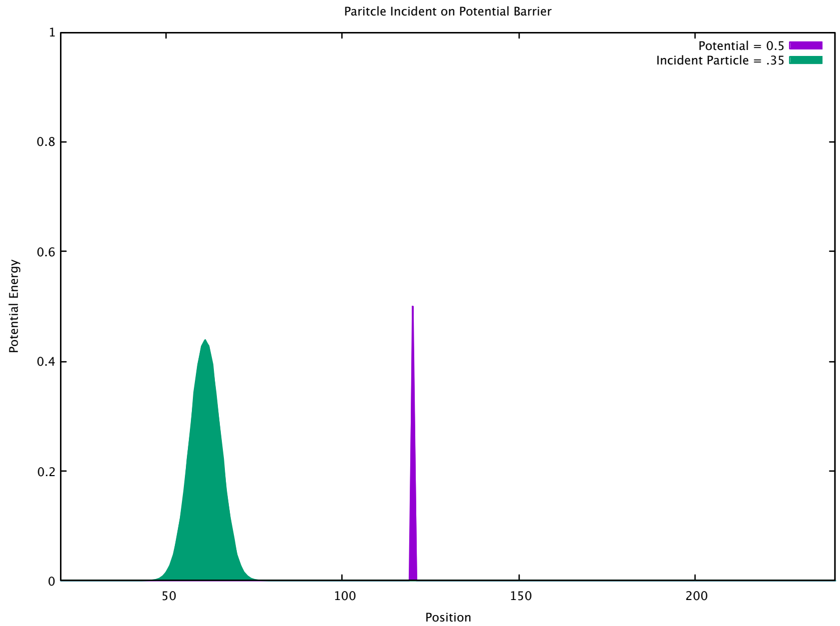

Figure 2: The particle initially sent in from the left before it interacts with the potential barrier

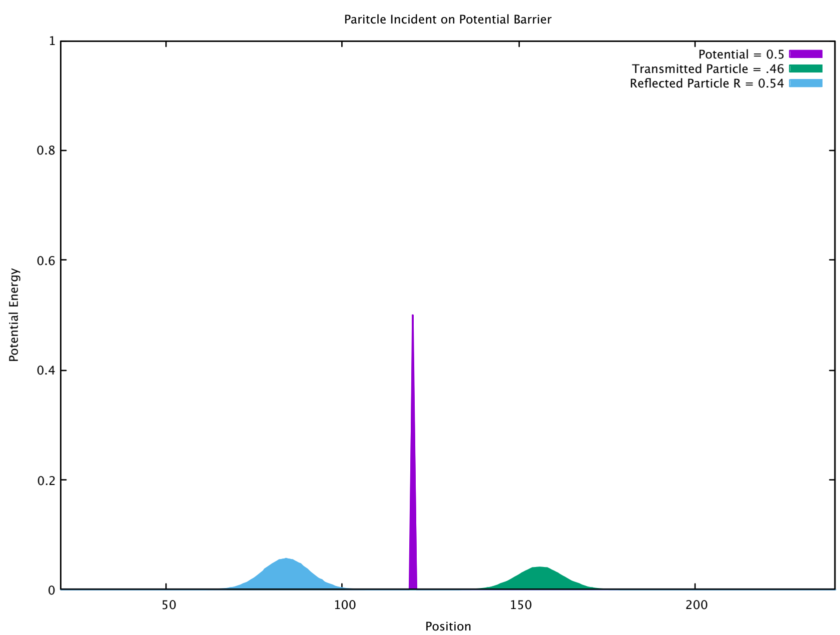

Figure 3: After having come in contact with the potential barrier the wave packet splits in to two components, a reflected and transmitted packet. The magnitude of the amplitude of each wave packet is proportional to the transmission and reflection coefficients calculated using the physical parameters of the potential barrier.

6 Discussion

Some future extensions that could be done to this program in the future would be coding in how the particle interacts with the potential barrier at the boundary. This behavior would take some thought and extra care when modeling, but would be fascinating and insightful when viewed. It would also be useful to program in a negative potential barrier, so that when the particle passes over it would be pulled down into the potential well.

Simulation programs such as this one are an important too for the physics community to come up with experiments that can be carrier out quickly, cheaply and timely. These programs are also good at allowing the simulation to be repeated multiple times. With many, easily changeable parameters many different outputs can be recorded and analyzed to be used in further modeling. Without these simulations certain certain experiments would not have the same repeatability or would be too costly and time consuming to get the same results as with a computer generated simulation.

References

[1] Donato, David, 2004, PHYS590 Study Guide: *The Potential Barrier - TUNNELING*, http://physics.gmu.edu/~dmaria/590%20Web%20Page/public_html/qm_topics/potential/barrier/STUDY-GUIDE.htm, 4/2/2017

[2] Griffiths, David J. (2004). Introduction to Quantum Mechanics (2nd ed.). Prentice Hall

[3] Alejandro L. Garcia, Numerical Methods for Physics (Prentice Hall, Englewood Cliffs NJ, 2000)

[4] PHYS 240 HW1

[5] Fitzpatrick, Richard, 2010-07-20 *Infinite Potential Well* http://farside.ph.utexas.edu/teaching/qmech/Quantum/node47.html#e5.6, 5/19/2017