Milestone Report 2

Tools thus far: numpy, differentiation by finite differences, midpoint quadrature, Diagonalization, Solving an eigenvalue problem.

Methodology/Progress Summary: I utilized my existing wavefunction example and utilized midpoint rule quadrature upon a for loop to integrate over each region of the well within certain intervals of time since the wavefunction is time dependent and is evolving. I then computed the maximum probability from the list of integral values as well as the time in which these maximums occurred. From this I graphically represented (this aspect is commented for now to improve the speed of the code) the probabilities of each region over time, as well as the graph of the maximum probability wavefunction at its specific time. I then converted this code to a set of functions so that I could input different parameters for the height and width of the barrier and see its effect upon maximum transmission likelihood. I then defined different variations of those functions that worked for simple gaussian wave packets, so that I could test the effect of the barrier on different distributions with different uncertainties, as well as a gaussian distribution generator. These new features will allow me to examine the weights of these features on transmissibility.

Challenges: The main issue that I ran into was the integration of regions over time, as it was difficult to navigate considering the time evolution of the probability distribution. In addition, I was unsure whether to consider maximum probability values that were the account of frequent reflections against boundaries and the barrier itself, I perhaps would want to make the size of the boundary greater so that there is enough precision to examine the wavefunction that is transmitted through the barrier. I am also having difficulty in picking barrier potential values that do not completely reflect the wave even with a small width. This will be examined further in my next milestone report.

A challenge that I overcame was properly indexing the wave function such that the probabilities summed to 1. I had a lot of issues before with double counting, as well as incorrect parsing through data points

Next Steps: Next, I will determine a way to quantify the effects of each parameter in my simulation on the transmissibility of the wave packet, either by utilizing statistical inference tools such as Bayesian Inference (determining transmission probability of a simulated wave packet subject to arbitrary parameters) , or ML tools such as scikit that perform feature analysis. With this I can begin examining the relative effects of these parameters and visualize them graphically.

Citations: *Griffiths, David J.; Schroeter, Darrell F. (2018). Introduction to quantum mechanics (3rd ed.). Cambridge: Cambridge University Press.,* https://www.dam.brown.edu/people/alcyew/handouts/numdiff.pdf