

Milestone Report 1

Tools thus far: numpy, differentiation by finite differences, midpoint quadrature,

Methodology/Progress Summary: To start I defined an arbitrary wavefunction evaluated at $t=0$ and defined within an interval (in this case this was $(-5,5)$). Utilizing formulations from Introduction to Quantum Mechanics, I defined a set of $N \times x$ values and computed this initial particle state at $t=0$. After normalizing, I found the hamiltonian matrix representation of this, by thinking of the x values as dividing the wave function $\psi(x,0)$ into elements and computing on paper the first and second derivatives of ψ by way of finite differences of each consecutive element of ψ (these mathematical calculations will be included on the Jupyter notebook in my final draft). That way I could substitute this into Schrodinger's Equation, and construct a matrix. I then utilized the `np.linalg.eigh()` function to compute the Eigen-energies and eigenvectors (stationary states) using the hamiltonian. I then normalized the eigenvectors. All that was left to do after this point was to calculate the coefficients so that I could start gauging probability using the formulas in Introduction to QM (I will reference the specific formulas in my final report). From there, I defined a simple manner of integration using the midpoint rule (I will experiment with others further along). The last portion of my progress which remains unfinished is the computation of integrals of the time dependent wave function over time, which I plan to compute the integrals of each region (left side of barrier, inside barrier, right side of barrier) from which I will find the minimum probability (while taking into account reflection) of the particle being on the left side of barriers. Then I can derive the probability of tunneling and compare this to the analytical solution found in the text book in terms of transmission coefficients.

Challenges: So far the main challenge is the resolution of midpoint integration (could introduce a lot of error as noise is introduced) and the effect of interference of reflecting and transmitting waves. Additionally I am currently struggling to compute integrals for each region, and I must make adjustments to my code in order to index the corresponding values in ψ with those in some interval in x .

Challenges that I overcame was figuring out how to create a matrix representation of some N dimensional matrix (indexed by elements x) which I was able to surpass through one of my sources ([dam.brown.edu](https://www.dam.brown.edu/people/alcyew/handouts/numdiff.pdf)) which allowed me to visualize how to split up the wavefunction into function evaluations at different x values.

Next Steps: In addition to what I briefly mentioned at the end of Methodology/Progress Summary, my next steps will be to establish an effective way to compute tunneling probability (by analyzing the error) through either different integration methods or some other solution. In addition, I will try to begin generating different parameters for different particles (I intend to begin generating a set of different wave function preparations and different barrier potentials/widths), and visualizing their tunneling probabilities against one another.

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>