Scattering

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Introduction

For our project, we created two simulations that serve as examples of how scattering states propagate using scattering matrices. These deal with a free particle moving in a potential of zero and then encountering an external potential. Specifically, we implemented a delta potential and a step potential. For each of these, we solved the Schrödinger equation $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$ for each side of the boundary using the boundary conditions that $\psi_1 = \psi_2$ at the boundary and $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ at the boundary.

The below sections describe each of the two simulations and the math involved with creating the,. An important thing to understand about the simulation is that the blue curve shows the real part of the solution and the yellow curve shows the imaginary part of the solution. Knowing this, the wave can be seen to “rotate” in the real and imaginary plane.

Delta Potential Simulation

When solving the delta potential, we have a potential of

$$V(x) = -\alpha\delta(x).$$

From here, the Schrödinger equation reads

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

The solution to this is

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2(x) = Fe^{ikx} + Ge^{-ikx}$$

Since we are simulating a particle coming from the left with no incident particle from the right, we have $G = 0$. Applying the boundary conditions discussed above, we have

$$A + B = F$$

$$F = (1 + 2i\beta) - (1 - 2i\beta)B$$

where $\beta = \frac{m\alpha}{\hbar^2 k}$

By turning this into a matrix we get

$$\begin{pmatrix} B \\ F \end{pmatrix} = S\begin{pmatrix} A \\ G \end{pmatrix}$$

$$S = \frac{1}{1-i\beta}\begin{pmatrix} i\beta & 1 \\ 1 & i\beta \end{pmatrix}$$

When creating our simulation, we used A=1. We used manipulate to allow the user to change the value of α. This changed the height of the delta potential. It can be seen that a higher α causes less transmission and more reflections. Additionally, the user could change the value of E, the incoming energy. This changed the wavelength and frequency of the wave.

We then implemented time dependence by multiplying each $\psi(x)$ by e^{-iwt} with w and k each being determined by E. By animating the plot with time, the user is able to see the wave function move as time progresses. They are also able to pause the simulation, speed it, or slow it.

Step Potential Simulation

When solving the step potential, we have a potential of

$$V(x) = \{ \begin{smallmatrix} 0 & x<0 \\ V & x>0 \end{smallmatrix}$$

The solution to this is

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$
$$\psi_2(x) = Fe^{ik_2x} + Ge^{-ik_2x}$$

Since we are simulating a particle coming from the left with no incident particle from the right, we have $G = 0$. Applying the boundary conditions discussed above, we have

$$A + B = F$$
$$ik_1A - ik_1B = ik_2F$$

By solving these equations we obtain

$$B = \frac{k_2-k_1}{k_2+k_1}$$
$$F = \frac{2k_1}{k_1+k_2}$$

As above, when creating our simulation, we used A=1. We used manipulate to allow the user to change the values of E and V. Changing E, the incoming energy, changes the wavelength and frequency of the incoming wave. Changing V changed the height of the potential step. It can be seen that when the energy is above the height of the potential step, the wave continues sinusoidally with some reflection and some transmission. When the energy is below the height of the potential step, tunnelling occurs. This reveals itself as a slight transmission in the form of an exponential decay with near perfect standing waves occurring due to reflection.

We then implemented time dependence by multiplying each $\psi(x)$ by e^{-iwt} with w and k each being determined by E. By animating the plot with time, the user is able to see the wave function move as time progresses. They are also able to pause the simulation, speed it, or slow it.