

# Scattering and quantum tunneling

## Introduction

In this exercise you are going to investigate scattering and tunneling in two different systems using the simulation tool Quantum Composer. The goal is to get a more intuitive understanding of the dynamics and behavior of a particle scattering on different potentials.

## Background

### System A

The first system, System A, describes the scattering of a free particle on a square barrier. The ground state of the free particle, a particle at rest, is described by the Gaussian wave

$$\psi_{\text{gs,A}} = e^{-\frac{(x-a)^2}{2b^2}},$$

where  $a$  is the initial position of the center of the wavefunction and  $b$  is the width of the Gaussian wave. To get the particle moving in Composer, it is given a momentum kick towards the scattering potential. This momentum kick is given by

$$\psi_k = e^{ikx},$$

where  $i$  is the imaginary unit and  $p = \hbar k$  is the momentum kick (we set  $\hbar = 1$  in Composer). The total wavefunction thus becomes

$$\psi_A = \psi_k \psi_{\text{gs,A}}. \tag{1}$$

The scattering potential is a smoothed square potential with variable height and width

$$V = \begin{cases} 0, & -\infty < x < a \\ U, & a < x < b \\ 0, & b < x < \infty \end{cases}.$$

An optional infinite potential can also be added at the edges

$$V_{\text{opt}} = \begin{cases} \infty, & -\infty < x < -c \\ 0, & -c < x < c \\ \infty, & c < x < \infty \end{cases}.$$

An example of this system can be seen in figure 1.

### System B

In the second system, System B, the potential is given by

$$V = \begin{cases} \infty, & -\infty < x < 0 \\ 0, & 0 < x < a \\ U_1, & a < x < b \\ U_2, & b < x < \infty \end{cases},$$

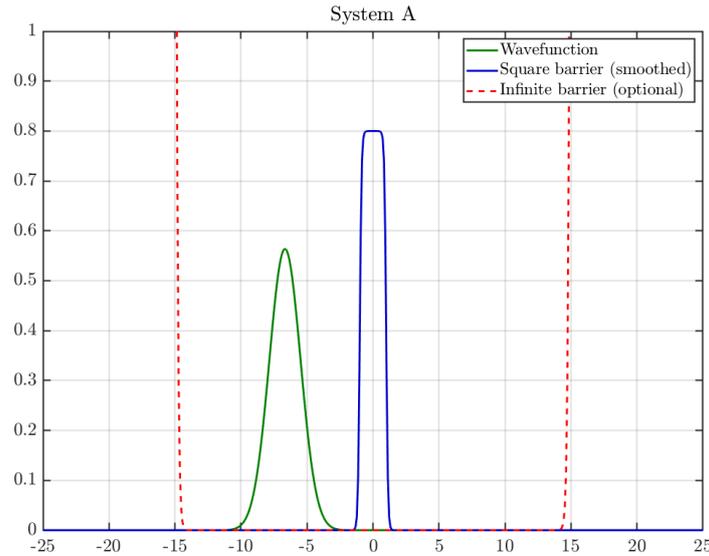


Figure 1: An example of system A. The potential of system can be seen in blue, the optional infinite barrier in red (dashed line) and the wavefunction in green.

with  $U_2 < U_1$  (default).

The wavefunction is the ground state of a particle trapped in the region  $0 < x < a$ . This ground state,  $\psi_{gs,B}$ , is difficult to analytically write down, so it is already calculated by Composer. To see the dynamics of the system, this ground state is also given a momentum kick as in Eq. 1, and this can be described mathematically as

$$\psi_B = \psi_k \psi_{gs,B}. \tag{2}$$

An example of this system can be seen in figure 2.

## The flowfile

The flowfiles for the exercise are called *scattering\_exercise\_A.flow* and *scattering\_exercise\_B.flow*, and refer System A and B respectively. As with any Composer work, it is highly recommended that you use a mouse to navigate the flowfile. The scene can be dragged around with a right click and zoomed in and out with the mouse wheel.

For both systems, the settings of the simulations are found to the left and the simulation plots can be seen to the right. The position plots show the spatial representation of the systems. The three plots beneath show the probability of measuring the particle to the left, in the middle (inside  $U$  for system A and  $U_1$  for system B) and to the right of the potential respectively. Beneath these plots, a numerical value of the probability can be found. Just to the left of the time evolution box are three nodes. These control the simulation duration and the size of the timesteps.

In System B an energy plot can also be seen. This shows the potential and the different states of the particle inside the potential. The number of eigenstates can be chosen at the top right corner. The ground state is the state shown for  $N_{eigenstates} = 1$ .

In both systems, the spatial dimension acts as a hard boundary, so if the particle hits the limits on either side ( $x_{min}$  and  $x_{max}$ ), there may be unintended reflections. To avoid this, either ignore the simulation results after these reflections or increase the spatial dimension.

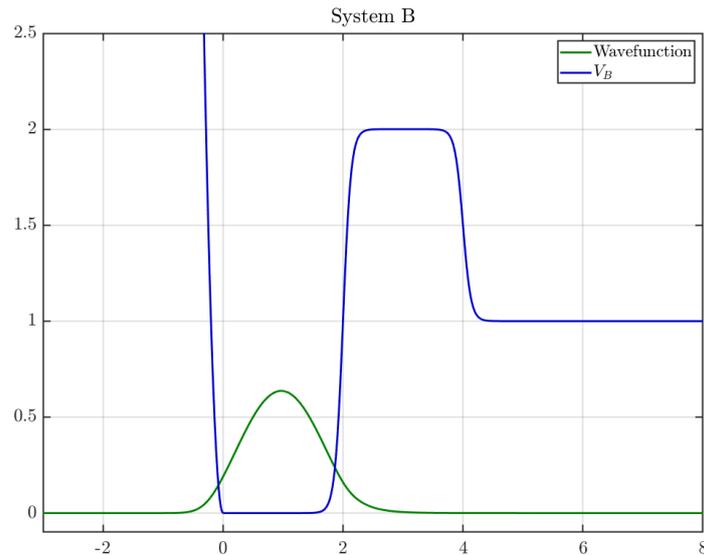


Figure 2: An example of system B. The potential can be seen in blue and the wavefunction in green.

## 1 Problem A

For each exercise, describe the simulation or the result in your own words.

1. Run the simulation (use the spacebar as a shortcut to run and pause, ctrl+r to reset the simulation), and look at the four plots. What happens? What are the maximum probabilities seen in each of the lower three graphs (roughly)?
2. Now that you have seen the system up close, you can increase the spatial dimension from -25 to 25, and the simulation time,  $tf$ , to 10. This lets the system evolve longer. If at any time you need to see the system up close, simply lower the spatial dimension again, but remember the hard boundaries!
3. Try increasing the barrier width to 4. To avoid that the particle starts partways into the barrier, move the particle to the left by setting  $x_0 = -5$ . Do you notice anything different from before?
4. Set the barrier width back to 2 and  $x_0 = -4$ . Try setting the barrier height to 10. What happens? How thin does the barrier have to be, to get at least a 25% probability of the wavefunction to be at the right of the barrier?
5. Change the barrier height back to 0.8 and the width to 2. Does changing the momentum kick,  $k$ , change the probabilities? How big does  $k$  have to be for the entire wavefunction to make it through (0.99 %) - what is the smallest  $k$  where it is possible? What happens when  $k$  is 0?
6. Set  $k = 1.5$ . Does changing  $x_0$  affect the probabilities? If yes, why do you think this is?
7. Set  $x_0 = -4$  and  $k = 1.5$ . Try setting the barrier height to -1 (the y-axis can be changed in the position plot). What happens? Do the probabilities at the end of the simulation change, if the height is reduced to -10? Can you find a value where there is less than 1 % probability at the right of the barrier (now a well) at the end of the simulation (ignoring artifacts from the boundaries)? Why/why not?

## 2 Problem B

For each exercise, describe the simulation or the result in your own words.

1. Look at the energy plot. Draw the potential on a piece of paper. Set  $N_{eigenstates}$  to 1 and draw the ground state. Now increase the number of eigenstates by one and draw the excited states, until you reach  $N_{eigenstates} = 4$ . If there were no momentum kick, which states do you think are bound?
2. Run the simulation, and look at the four plots. What happens? Increase  $x_{max}$  to 16 (it makes it easier to see the probabilities properly, without any boundary artifacts). What are the maximum probabilities seen in each of the lower three graphs (roughly)?
3. Try increasing the value of  $U_2$ . What happens to the potential? What happens in the simulation?
4. Set  $U_2$  back to 1. Increase the barrier length. How do the probabilities change? How long does the barrier have to be for the probability at the right to be less than 5% at the end of the simulation? What happens to the probability in the well (at the left) with these settings?
5. Set the length back to 2 and increase the height to 10. What happens to the left probability? How much makes it through the barrier?
6. Set the height back to 2. How high does  $k$  have to be for at least 99 % of the wavefunction to make it through the barrier before boundary artifacts kick in?

## Conclusion

You are now welcome to explore both simulations as you wish. What other interesting behaviour can you uncover?

In system A, you can edit the following nodes:

- $x_{min}$ , the start of the spatial dimension
- $x_{max}$ , the end of the spatial dimension
- $n$ , the number of spatial grid points (ideal values are  $n = 2^m$ , where  $m$  is an integer)
- box limits, the limits of the optional infinite potential (30 by default)
- barrier center, the center of the potential barrier
- barrier width, the width of the potential barrier
- barrier height, the height of the potential barrier
- $x_0$ , the initial center of the wavefunction
- width, the initial width of the wavefunction
- $k$ , the momentum kick of the wavefunction
- $tf$ , the length of the simulation
- $dt$ , the number of simulated timesteps (lower values gives a more precise but also slower simulation).

In system B, you can edit the following nodes:

- $x_{max}$ , the end of the spatial dimension
- $n$ , the number of spatial grid points (ideal values are  $n = 2^m$ , where  $m$  is an integer)
- barrier start, the start of the potential barrier
- barrier length, the length of the potential barrier
- barrier height, the height of the potential barrier

- $U_2$ , the value of the asymptotic potential at the right of the barrier
- $k$ , the momentum kick of the wavefunction ( $p = \hbar k$  is the momentum kick, but  $\hbar = 1$  in Composer)
- $t_f$ , the length of the simulation
- $dt$ , the number of simulated timesteps (lower values gives a more precise but also slower simulation).

All the other nodes should be left untouched.

