# EXERCISE 19

# Solving the Schrödinger equation for the step potential

Solve the time-independent Schrödinger equation,

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

for the step potential

$$V(x) = \begin{cases} 0 & \text{if} \quad x < 0 \\ V_0 & \text{if} \quad x > 0 \end{cases}\,.$$

Throughout this exercise, assume that $V_0 > 0$.

Specifically, show that when the energy $E$ is lower than the step height $V_0$, the solution is given by

$$\psi(x) = \begin{cases} e^{ikx} + \frac{k-ik'}{k+ik'}e^{-ikx} & \text{if} \quad x < 0 \\ \frac{2k}{k+ik'}e^{-k'x} & \text{if} \quad x > 0 \end{cases}\,.$$

Conversely, if the energy $E$ is higher than $V_0$, then

$$\psi(x) = \begin{cases} e^{ikx} + \frac{k-k''}{k+k''}e^{-ikx} & \text{if} \quad x < 0 \\ \frac{2k}{k+k''}e^{ik''x} & \text{if} \quad x > 0 \end{cases}\,.$$

In the expressions above,

$$k = \frac{\sqrt{2mE}}{\hbar}\,, \quad k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}\,, \quad k' = \frac{\sqrt{2m(E - V_0)}}{\hbar}\,.$$

# Solution

## Case $\boxed{E < V_0}$

- For $\boxed{x < 0}$ the Schrödinger equation reads

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

  or

  $$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0\,,$$

  where

  $$k = \frac{\sqrt{2mE}}{\hbar}\,.$$

  The general (up to an overall constant multiplier) solution can be written as

  $$\psi(x) = e^{ikx} + Be^{-ikx}\,. \tag{1}$$

  Here, $e^{ikx}$ represents an incident plane wave moving from left to right, towards the potential step, and $e^{-ikx}$ represents a reflected plane wave moving from right to left, away from the step. For convenience, we choose the amplitude of the incident plane wave to be 1. The amplitude of the reflected wave, $B$, is so far an arbitrary complex number.

- For $\boxed{x > 0}$ the Schrödinger equation reads

  $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x)\,,$$

  or

  $$\frac{d^2\psi(x)}{dx^2} - k'^2\psi(x) = 0\,,$$

  where

  $$k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}\,.$$

  The general solution is

  $$\psi(x) = Ce^{-k'x} + De^{k'x}\,,$$

  where $C$ and $D$ are arbitrary constants.

  Notice that the function $e^{k'x}$ increases rapidly (exponentially!) as $x$ increases and diverges as $x \to +\infty$. Keeping this function in the solution to the Schrödinger equation would lead to an unphysical scenario where the particle would be predominantly present at infinity, making the overall state non-normalizable. To keep the solutions physically meaningful, we have to set $D = 0$, which leaves us with

  $$\psi(x) = Ce^{-k'x}\,. \tag{2}$$

- At $\boxed{x = 0}$ the wave function has to satisfy the so-called matching conditions: it has to be continuous and differentiable. This means that constants $B$ and $C$ have to be such that

$$\psi(-0) = \psi(+0)\,,$$

$$\frac{d\psi}{dx}(-0) = \frac{d\psi}{dx}(+0)\,.$$

Here, the argument $-0$ (respectively, $+0$) means that the corresponding function is evaluated just to the left (respectively, just to the right) of $x = 0$. In other words, we need to use Eq. (1) for calculating $\psi(-0)$ and $\frac{d\psi}{dx}(-0)$, and Eq. (2) for calculating $\psi(+0)$ and $\frac{d\psi}{dx}(+0)$. Doing this, we get the following system of equations:

$$1 + B = C\,,$$

$$ik - ikB = -k'C\,.$$

The solution to the system is given by

$$B = \frac{k - ik'}{k + ik'} \quad \text{and} \quad C = \frac{2k}{k + ik'}\,. \tag{3}$$

Combining Eqs. (1), (2), and (3), we obtain the sought solution:

$$\psi(x) = \begin{cases} e^{ikx} + \frac{k-ik'}{k+ik'}e^{-ikx} & \text{if} \quad x < 0 \\ \frac{2k}{k+ik'}e^{-k'x} & \text{if} \quad x > 0 \end{cases}\,.$$

## Case $\boxed{E > V_0}$

- For $\boxed{x < 0}$ the analysis is exactly the same as in the $E < V_0$ case. So, the solution in this region is, as before, given by

$$\psi(x) = e^{ikx} + Be^{-ikx} \tag{4}$$

with $B$ being some yet-to-be-determined constant.

- For $\boxed{x > 0}$ the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x)\,,$$

or

$$\frac{d^2\psi(x)}{dx^2} + k''^2\psi(x) = 0\,,$$

where

$$k'' = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

The general solution is

$$\psi(x) = Ce^{ik''x} + De^{-ik''x},$$

where $C$ and $D$ are arbitrary constants.

The function $e^{ik''x}$ represents a plane wave transmitted over the potential step and traveling to the right, away from the step. This part of the solution is physically meaningful. The function $e^{-ik''x}$, however, corresponds to a plane wave moving from right to left, from $+\infty$ towards the potential step. But in the scenario considered here, there should be only one incident wave, and it should approach the potential step from $-\infty$, not from $+\infty$. Therefore, the only way to resolve this apparent inconsistency is to set the amplitude of $e^{-ik''x}$ to zero. So, setting $D = 0$, we get

$$\psi(x) = Ce^{ik''x}. \tag{5}$$

- At $\boxed{x = 0}$ the matching conditions require that

$$\psi(-0) = \psi(+0),$$

$$\frac{d\psi}{dx}(-0) = \frac{d\psi}{dx}(+0).$$

Using Eq. (4) for calculating $\psi(-0)$ and $\frac{d\psi}{dx}(-0)$, and Eq. (5) for calculating $\psi(+0)$ and $\frac{d\psi}{dx}(+0)$, we obtain the following system of equations for $B$ and $C$:

$$\begin{aligned} &1 + B = C, \\ &ik - ikB = ik''C. \end{aligned}$$

The solution to this system is given by

$$B = \frac{k - k''}{k + k''} \quad \text{and} \quad C = \frac{2k}{k + k''}. \tag{6}$$

Combining Eqs. (4), (5), and (6), we obtain

$$\psi(x) = \begin{cases} e^{ikx} + \frac{k-k''}{k+k''}e^{-ikx} & \text{if} \quad x < 0 \\ \frac{2k}{k+k''}e^{ik''x} & \text{if} \quad x > 0 \end{cases}.$$