

The Schrödinger Equation

We have previously considered the wave function $\psi(x, t)$ and its analogy to plane waves.

$$\psi(x, t) = A \cdot e^{i(kx - \omega t)} = A \cdot e^{\frac{i}{\hbar}(px - Et)},$$

Our considerations revealed that plane waves are good elementary waves but not suitable for describing particles, which are localized in space. In order to describe particles, we have to consider wave packets, which are superpositions of plane waves.

We would like to obtain now a differential equation that governs the time evolution of the wave function $\psi(x, t)$. We start from the fundamental principle of energy conservation in classical mechanics:

$$E = E_{\text{kin}} + E_{\text{pot}}$$

For a particle of mass m : $E = \frac{p^2}{2m} + V(x)$

To transition to quantum mechanics, we combine the plane wave description of the wave function with the energy conservation principle: If we apply the following differential operators to the wave function $\psi(x, t)$:

- Energy: $E \rightarrow i\hbar \frac{\partial}{\partial t}$
- Momentum: $p \rightarrow -i\hbar \frac{\partial}{\partial x}$

we obtain the time-dependent Schrödinger equation in one dimension:

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x) \psi$$

This is the time-dependent Schrödinger equation in one dimension. It looks different from a wave equation, but it is a wave equation. The time-dependent Schrödinger equation is a wave equation for the wave function $\psi(x, t)$, that shall describe the flow of probability density in space and time.

i Why First-Order in Time?

From optics, we are used to the wave equation containing a second order time derivative. This is not existing in the time dependent Schrödinger equations, which is supposed to be a wave equation as well. To understand why the Schrödinger equation contains only a first-order time derivative, let us compare three fundamental equations in physics: The classical wave equation involves a second time derivative:

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}$$

The diffusion equation contains a first-order time derivative with real coefficients:

$$\frac{\partial \psi}{\partial t} = D \frac{\partial^2 \psi}{\partial x^2}$$

The Schrödinger equation has a first-order time derivative with a complex coefficient:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

A key requirement for quantum mechanics is the conservation of probability, expressed mathematically as

$$\frac{d}{dt} \int |\psi|^2 dx = 0$$

Let us examine this condition for the Schrödinger equation:

$$\frac{d}{dt} \int |\psi|^2 dx = \int (\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}) dx$$

Using the Schrödinger equation and its complex conjugate:

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \\ -i\hbar \frac{\partial \psi^*}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} \end{aligned}$$

The terms cancel exactly, giving $\frac{d}{dt} \int |\psi|^2 dx = 0$. This conservation of probability does not hold for the diffusion equation, where $\frac{d}{dt} \int |\psi|^2 dx \neq 0$. Furthermore, a second-order time derivative would not preserve the phase relationships necessary for quantum interference.

The complex nature of the Schrödinger equation, particularly the imaginary unit ‘i’, is therefore essential for maintaining probability conservation, enabling wave-like solutions, and preserving quantum phase relationships.

Stationary Schrödinger Equation

For states with definite energy (stationary states), we can separate the time dependence using:
 $\psi(x, t) = \psi(x)e^{-iEt/\hbar}$

Inserting this into the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x)\psi$$

The time derivative gives $E\psi$ on the left side, leading to the stationary Schrödinger equation:

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

This is the stationary Schrödinger equation in one dimension. It is a wave equation for the wave function $\psi(x)$, that shall describe the spatial distribution of probability density. It compares to the Helmholtz equation in optics. Therefore, solutions we have found for the Helmholtz equation can be applied to the Schrödinger equation as well.

Solutions of the Schrödinger equation

To solve the stationary Schrödinger equation, we should take care of a number of boundary conditions:

1. The wave function $\psi(x)$ must be continuous.
2. The first derivative of the wave function $\frac{\partial \psi}{\partial x}$ must be continuous.
3. The wave function $\psi(x)$ must be square integrable, i.e. $\int |\psi(x)|^2 dx < \infty$.

These are the main conditions, which help us to solve the Schrödinger equation. We will now discuss some examples of solutions of the Schrödinger equation.

A potential barrier

Let's consider a quantum particle encountering a potential step: for $x < 0$, the potential $V(x) = 0$, while for $x \geq 0$, $V(x) = E_0$. This is similar to a light wave hitting the interface between two different materials.

To solve this problem, we need to look at two regions separately and match their solutions at $x = 0$.

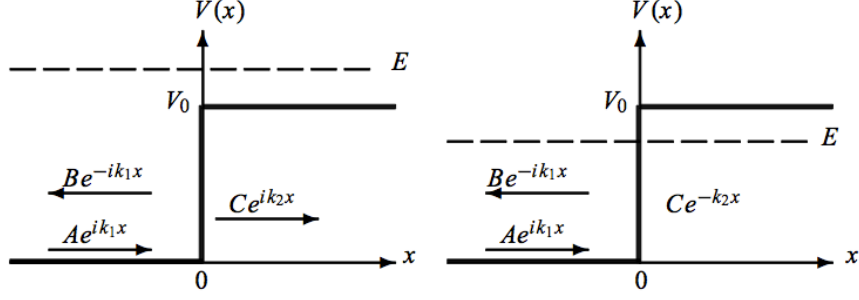


Figure 1: Sketch of the potential barrier. A wave with a kinetic energy E_{kin} approaches a potential barrier E_0 with $E_0 > E_{\text{kin}}$. The wave is completely reflected (amplitudes $|A| = |B|$), but intrudes the barrier where the amplitude decays exponentially.

Region 1 - $x < 0$:

In the first region where $V = 0$, the stationary Schrödinger equation is:

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

The solution is a combination of incoming and reflected waves:

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

where $k = \sqrt{2mE}/\hbar$

Region 2 - $x \geq 0$:

In the second region where $V = V_0$, the Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V_0\psi = E\psi$$

The solution here is:

$$\psi_2(x) = Ce^{\alpha x} + De^{-\alpha x}$$

where $\alpha = \sqrt{2m(V_0 - E)}/\hbar$

To connect these solutions, we need two boundary conditions at $x = 0$:

1. The wave function must be continuous:

$$A + B = C + D$$

2. Its derivative must be continuous:

$$ik(A - B) = \alpha(C - D)$$

The case $E < V_0$

In the case $E < V_0$, α is real and we set $C = 0$ to prevent ψ_2 diverging as $x \rightarrow \infty$. The boundary conditions give:

$$B = \frac{ik + \alpha}{ik - \alpha} A$$
$$D = \frac{2ik}{ik - \alpha} A$$

The wave function in region 1 ($x < 0$) is:

$$\psi_1(x) = A \left(e^{+ikx} + \frac{ik + \alpha}{ik - \alpha} e^{-ikx} \right).$$

The reflection coefficient, comparing reflected and initial wave intensities, is:

$$R = \frac{|B \cdot e^{-ikx}|^2}{|A \cdot e^{+ikx}|^2} = \frac{|ik + \alpha|^2}{|ik - \alpha|^2} = 1.$$

This shows total reflection, as expected for $E < V_0$. However, quantum mechanics reveals that particles still penetrate slightly into region 2 ($x \geq 0$).

```
hbar = 1.0
m = 1.0
V0 = 1.0
E = 0.5 # Energy less than V0
A = 0.3 # Incident amplitude (reduced for clarity)

# Wave numbers
k = np.sqrt(2*m*E)/hbar
alpha = np.sqrt(2*m*(V0 - E))/hbar

# Coefficients
```

```

B = (1j*k + alpha)/(1j*k - alpha) * A
D = 2*1j*k/(1j*k - alpha) * A

# Position arrays
x1 = np.linspace(-10, 0, 1000) # Region 1
x2 = np.linspace(0, 10, 1000)   # Region 2

# Wavefunctions (offset by energy E)
psi1 = A * np.exp(1j*k*x1) + B * np.exp(-1j*k*x1) + E
psi2 = D * np.exp(-alpha*x2) + E

# Potential step
V = np.zeros_like(np.concatenate([x1, x2]))
V[len(x1):] = V0

plt.figure(figsize=get_size(12, 6))
# Plot potential
plt.plot(np.concatenate([x1, x2]), V, 'k-', label='Potential V(x)')
# Plot wavefunctions
plt.plot(x1, np.real(psi1), 'b-', label='Region 1')
plt.plot(x2, np.real(psi2), 'r-', label='Region 2')

# Add vertical line at boundary
plt.axvline(x=0, color='k', linestyle='--', alpha=0.5)
plt.axhline(y=0, color='k', linestyle='-', alpha=0.3)
plt.axhline(y=0.5, color='k', linestyle='--', alpha=0.3)

plt.xlabel('position x')
plt.ylabel('energy')
plt.legend()
plt.ylim(-0.2, 1.2)
plt.show()

```

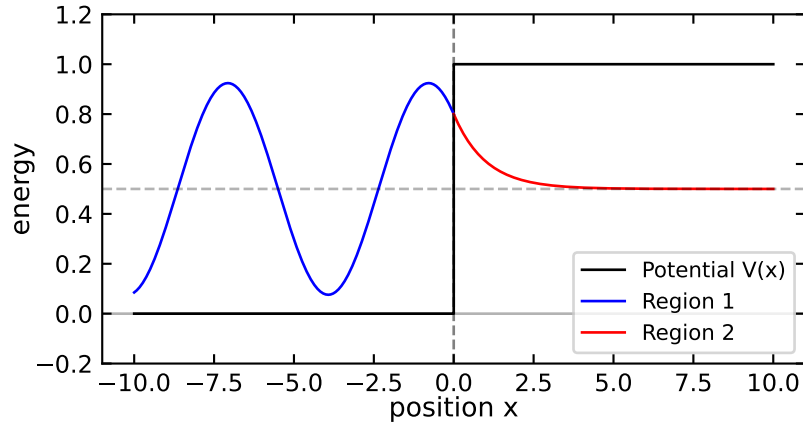


Figure 2: Plot the wavefunctions for $E < V_0$

The probability density $P(x)$ for $x > 0$ is:

$$P(x) = |\psi_2(x)|^2 = |D \cdot e^{-\alpha x}|^2 = \frac{4k^2}{\alpha^2 + k^2} e^{-2\alpha x} = \frac{4k^2}{k_0^2} e^{-2\alpha x},$$

where $k^2 = 2mE/\hbar^2$ and $k_0^2 = 2mV_0/\hbar^2$. At $x = 1/(2\alpha)$, the probability density drops to $1/e$ of its value at $x = 0$, similar to evanescent waves in total internal reflection. This is plotted below and demonstrates that there is still a small probability of finding the particle in region 2, even when $E < V_0$, which is later the basis for tunneling.

```
# Parameters
hbar = 1.0
m = 1.0
V0 = 1 # Fixed energy
E = np.linspace(0, V0-1e-2, 1000) # Range of potential values

# Calculate decay length
decay_length = 1/(2*np.sqrt(2*m*(V0 - E))/hbar)

plt.figure(figsize=get_size(12, 6))
plt.plot(V0-E, decay_length, 'b-')
plt.xlabel('V - E')
plt.ylabel('Decay Length 1/(2)')
plt.grid(True, alpha=0.3)
plt.show()
```

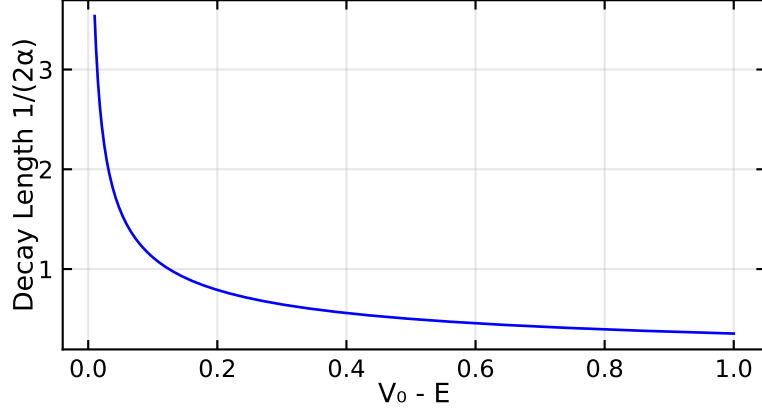


Figure 3: Decay length as a function of potential barrier height minus energy

The case $E > V_0$

When $E > V_0$, particles can classically enter region 2 with reduced kinetic energy $E_{kin} = E - V_0$. In quantum mechanics, α becomes imaginary, so we define a real wave number:

$$\kappa = i\alpha = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

The wave function in region 2 becomes:

$$\psi_2(x) = C \cdot e^{-i\kappa x} + D \cdot e^{+i\kappa x},$$

with $\psi_1(x)$ unchanged from before.

The boundary conditions at $x = 0$ require:

$$\begin{aligned} \psi_1(x=0) &= \psi_2(x=0) \\ \rightarrow A + B &= C + D \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial x} \psi_1(x=0) &= \frac{\partial}{\partial x} \psi_2(x=0) \\ \rightarrow ik(A - B) &= -i\kappa C + i\kappa D. \end{aligned}$$

Since no wave reflects from infinity, $C = 0$. This gives:

$$B = \frac{k - \kappa}{k + \kappa} A$$

$$D = \frac{2k}{k + \kappa} A$$

resulting in:

$$\psi_1(x) = A \left(e^{+ikx} + \frac{k - \kappa}{k + \kappa} e^{-ikx} \right)$$

$$\psi_2(x) = A \frac{2k}{k + \kappa} e^{+i\kappa x}.$$

The plot below shows the wave functions for $E > V_0$. The wave function in region 2 is oscillatory, indicating that the particle can penetrate the barrier region.

```
hbar = 1.0
m = 1.0
V0 = 1.0
E = 1.5 # Energy greater than V0
A = 0.3 # Incident amplitude (reduced for clarity)

# Wave numbers
k = np.sqrt(2*m*E)/hbar
kappa = np.sqrt(2*m*(E - V0))/hbar # Changed from alpha to kappa for E > V0

# Coefficients
B = (k - kappa)/(k + kappa) * A # Modified for E > V0
D = 2*k/(k + kappa) * A # Modified for E > V0

# Position arrays
x1 = np.linspace(-10, 0, 1000) # Region 1
x2 = np.linspace(0, 10, 1000) # Region 2

# Wavefunctions (offset by energy E)
psi1 = A * np.exp(1j*k*x1) + B * np.exp(-1j*k*x1) + E
psi2 = D * np.exp(1j*kappa*x2) + E # Changed to oscillatory solution

# Potential step
V = np.zeros_like(np.concatenate([x1, x2]))
V[len(x1):] = V0

plt.figure(figsize=get_size(12, 6))
```

```

# Plot potential
plt.plot(np.concatenate([x1, x2]), V, 'k-', label='Potential V(x)')
# Plot wavefunctions
plt.plot(x1, np.real(psi1), 'b-', label='Region 1')
plt.plot(x2, np.real(psi2), 'r-', label='Region 2')

# Add vertical line at boundary
plt.axvline(x=0, color='k', linestyle='--', alpha=0.5)
plt.axhline(y=0, color='k', linestyle='--', alpha=0.3)
plt.axhline(y=E, color='k', linestyle='--', alpha=0.3)

plt.xlabel('position x')
plt.ylabel('energy')
plt.legend()
plt.ylim(-0.2, 2.0)
plt.show()

```

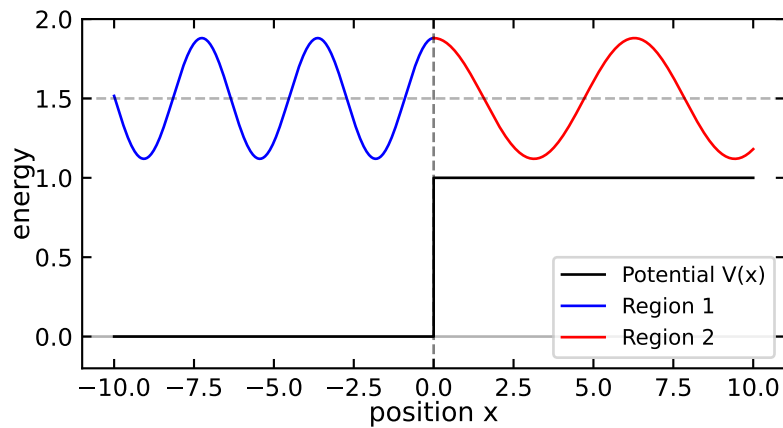


Figure 4: Plot the wavefunctions for $E > V_0$

Let's understand what these coefficients mean physically. The reflection coefficient R represents the probability that an incoming particle will be reflected at the potential barrier. We calculate it by comparing the squared magnitudes of the reflected wave (B) to the incident wave (A):

$$R = \frac{|B|^2}{|A|^2} = \frac{|k - \kappa|^2}{|k + \kappa|^2}$$

This expression is analogous to the reflection of light at an interface between two media with different refractive indices ($k = n_1 k_0$, $\kappa = n_2 k_0$):

$$R = \frac{|n_1 - n_2|^2}{|n_1 + n_2|^2}.$$

The transmission coefficient T tells us the probability that a particle will pass through the barrier. Because the particle velocities are different on either side of the barrier ($v_2/v_1 = k/\kappa$), we must account for this in our calculation:

$$T = \frac{v_1 \cdot |D|^2}{v_2 \cdot |A|^2} = \frac{4\kappa k}{(k + \kappa)^2}.$$

Since every particle must either reflect or transmit, these probabilities must sum to one:

$$R + T = 1.$$

When the particle's energy exactly equals the barrier height ($E = V_0$), both α and κ become zero, resulting in total reflection ($R = 1$). The plot below shows the trans

```
# Parameters
hbar = 1.0
m = 1.0
V0 = 1.0
E = np.linspace(V0, 5*V0, 1000) # Energy range from V0 to 2*V0

# Wave numbers
k = np.sqrt(2*m*E)/hbar
kappa = np.sqrt(2*m*(E - V0))/hbar

# Calculate coefficients
R = ((k - kappa)/(k + kappa))**2
T = 4*k*kappa/((k + kappa)**2)

plt.figure(figsize=get_size(10,8))
plt.plot(E/V0, R, 'b-', label='Reflection R')
plt.plot(E/V0, T, 'r-', label='Transmission T')
plt.plot(E/V0, R + T, 'k--', label='R + T = 1', alpha=0.5)

plt.xlabel('E/V ')
plt.ylabel('Coefficient')
plt.legend()
plt.grid(True, alpha=0.3)
plt.show()
```

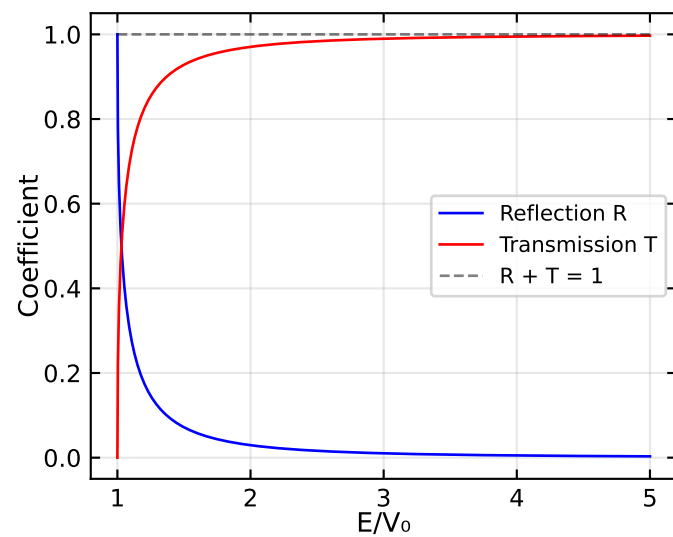


Figure 5: Transmission and reflection coefficients as functions of energy