Transmission Through a One–Dimensional Potential Barrier

General Formulation

We consider the time–independent Schrödinger equation

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

This equation may be written in the compact form

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

where the local wave number is defined by

$$\boxed{k^2(x) = \frac{2m}{\hbar^2}\,[E - V(x)].}$$

For regions where $E > V(x)$, $k(x)$ is real and the solutions are oscillatory. For regions where $E < V(x)$, $k(x)$ is imaginary and the solutions are exponential. Thus, a single definition of $k(x)$ suffices for all regions.

Potential Profile

We consider a finite barrier of width $2a$,

$$V(x) = \begin{cases} 0, & x < -a, \\ V_0, & |x| \le a, \\ 0, & x > a. \end{cases}$$

Accordingly,

$$k(x) = \begin{cases} k = \sqrt{\dfrac{2mE}{\hbar^2}}, & x < -a \text{ and } x > a, \\ i\kappa, \quad \kappa = \sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}, & |x| \le a. \end{cases}$$

Functional Form of the Wavefunction

Region I: $x < -a$ The wavefunction is a superposition of incident and reflected waves,

$$\boxed{\psi_I(x) = Ae^{ikx} + Be^{-ikx}.}$$

Its derivative is

$$\psi_I'(x) = ikAe^{ikx} - ikBe^{-ikx}.$$

In matrix form,

$$\begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = \begin{pmatrix} e^{ikx} & e^{-ikx} \\ ike^{ikx} & -ike^{-ikx} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}.$$

Region II: $|x| \leq a$ Inside the barrier, the wavefunction is

$$\boxed{\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}.}$$

Its derivative is

$$\psi_{II}'(x) = \kappa Ce^{\kappa x} - \kappa De^{-\kappa x}.$$

This may be written as

$$\begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = \begin{pmatrix} e^{\kappa x} & e^{-\kappa x} \\ \kappa e^{\kappa x} & -\kappa e^{-\kappa x} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}.$$

Region III: $x > a$ Only a transmitted wave exists,

$$\boxed{\psi_{III}(x) = Fe^{ikx}.}$$

Its derivative is

$$\psi_{III}'(x) = ikFe^{ikx}.$$

This may be written as

$$\begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = \begin{pmatrix} e^{ikx} & e^{-ikx} \\ ike^{ikx} & -ike^{-ikx} \end{pmatrix} \begin{pmatrix} F \\ 0 \end{pmatrix}.$$

Chain of 2×2 Matrices

By enforcing the continuity of $\psi(x)$ and $\psi'(x)$ at $x = -a$ and $x = +a$, the coefficients

$$(A, B) \longleftrightarrow (C, D) \longleftrightarrow (F, 0)$$

are related through a chain of 2×2 matrices.

Since all matrices are of order 2×2, the system may be solved systematically by matrix inversion and multiplication.

Numerical Solution Using the Euler Method

Instead of solving the matching conditions analytically, we solve the Schrödinger equation numerically.

We rewrite the second–order equation as two first–order equations:

$$\frac{d\psi}{dx} = \phi, \qquad \frac{d\phi}{dx} = -k^2(x)\psi.$$

Using the Euler method with step size h,

$$\boxed{\psi_{n+1} = \psi_n + h\,\phi_n,}$$

$$\boxed{\phi_{n+1} = \phi_n - h\,k^2(x_n)\psi_n.}$$

Determination of Coefficients from Local Linear Systems

the wavefunction $\psi(x)$ and its derivative $\psi'(x)$ are already known at the boundary points $x = -a$ and $x = +a$ from a numerical integration (Euler method).

The coefficients in each region are obtained by solving simple 2×2 linear systems of the form

$$\mathbf{AX} = \mathbf{B}.$$

No global transfer matrix or closed–form transmission formula is used.

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Region I Coefficients A, B at $x = -a$

In Region I,

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

Evaluating at $x = -a$,

$$\begin{pmatrix} e^{-ika} & e^{ika} \\ ike^{-ika} & -ike^{ika} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \psi(-a) \\ \psi'(-a) \end{pmatrix}.$$

Solving this system gives

$$\boxed{A = \frac{1}{2}\left[\psi(-a) + \frac{1}{ik}\psi'(-a)\right] e^{ika},}$$

$$\boxed{B = \frac{1}{2}\left[\psi(-a) - \frac{1}{ik}\psi'(-a)\right] e^{-ika}.}$$

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Region II Coefficients C, D at $x = -a$

Inside the barrier,

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}.$$

At $x = -a$,

$$\begin{pmatrix} e^{-\kappa a} & e^{\kappa a} \\ \kappa e^{-\kappa a} & -\kappa e^{\kappa a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \psi(-a) \\ \psi'(-a) \end{pmatrix}.$$

Solving,

$$\boxed{C = \frac{1}{2}\left[\psi(-a) + \frac{1}{\kappa}\psi'(-a)\right] e^{\kappa a},}$$

$$\boxed{D = \frac{1}{2}\left[\psi(-a) - \frac{1}{\kappa}\psi'(-a)\right] e^{-\kappa a}.}$$

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Region II Coefficients C, D at $x = +a$

Using the numerical solution at $x = +a$,

$$\begin{pmatrix} e^{\kappa a} & e^{-\kappa a} \\ \kappa e^{\kappa a} & -\kappa e^{-\kappa a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \psi(+a) \\ \psi'(+a) \end{pmatrix}.$$

Thus,

$$\boxed{C = \frac{1}{2}\left[\psi(+a) + \frac{1}{\kappa}\psi'(+a)\right] e^{-\kappa a},}$$

$$\boxed{D = \frac{1}{2}\left[\psi(+a) - \frac{1}{\kappa}\psi'(+a)\right] e^{\kappa a}.}$$

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Region III Coefficient F at $x = +a$

In Region III,

$$\psi_{III}(x) = Fe^{ikx}.$$

At $x = +a$,

$$\begin{pmatrix} e^{ika} \\ ike^{ika} \end{pmatrix} F = \begin{pmatrix} \psi(+a) \\ \psi'(+a) \end{pmatrix}.$$

This gives

$$\boxed{F = \psi(+a)\, e^{-ika},}$$

with consistency requiring

$$\psi'(+a) = ik\, \psi(+a).$$

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Extraction of Transmission Probability

Once the coefficient F is obtained from the numerical solution, the transmission probability is computed directly from the ratio of probability currents,

$$T = \frac{|F|^2}{|A|^2}.$$

Now , we plot the Transmission probability T as a function of Energy E