Quantum Tunneling through a Single Potential Barrier: Equivalence of the Transfer Matrix and Analytical Solutions

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Problem Setup

Suppose the potential $V(x)$ is given by:

$$V(x) = \begin{cases} V_0, & 0 \leq x \leq L \\ 0, & \text{otherwise} \end{cases}$$

We analyze the case for a particle with energy $E > 0$ incident from the left. This paper focuses on the quantum tunneling, so we assume the particle's energy is less than the barrier height: $0 < E < V_0$.

The Time-independent Schrödinger equation is:

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

Wave Function Solutions in Each Region

We define $k_1^2 = \frac{2mE}{\hbar^2}$ and $k_2^2 = \frac{2m(V_0-E)}{\hbar^2}$.

- **Region I ($x < 0, V = 0$):**

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

- **Region II ($0 \leq x \leq L, V = V_0$):**

$$\psi_{II}(x) = Ce^{k_2x} + De^{-k_2x}$$

- **Region III ($x > L, V = 0$):**

$$\psi_{III}(x) = Fe^{ik_1x}$$

Boundary Conditions

We apply continuity for $\psi(x)$ and $\frac{d\psi}{dx}$ at both $x = 0$ and $x = L$. This gives four conditions:

$$\psi_I(0) = \psi_{II}(0) \implies A + B = C + D \tag{1}$$

$$\psi_{II}(L) = \psi_{III}(L) \implies Ce^{k_2 L} + De^{-k_2 L} = Fe^{ik_1 L} \tag{2}$$

$$\left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0} \implies ik_1(A - B) = k_2(C - D) \tag{3}$$

$$\left.\frac{d\psi_{II}}{dx}\right|_{x=L} = \left.\frac{d\psi_{III}}{dx}\right|_{x=L} \implies k_2(Ce^{k_2 L} - De^{-k_2 L}) = ik_1 Fe^{ik_1 L} \tag{4}$$

Method 1: Analytical Approach (Solving the System)

Solving the system of four equations leads to expressions for the coefficients. By solving (2) and (4) for C and D:

$$C = \left(1 + \frac{ik_1}{k_2}\right)\frac{F}{2}e^{ik_1 L - k_2 L} \tag{5}$$

$$D = \left(1 - \frac{ik_1}{k_2}\right)\frac{F}{2}e^{ik_1 L + k_2 L} \tag{6}$$

And by solving (1) and (3) for A and B:

$$A = \left(1 - \frac{ik_2}{k_1}\right)\frac{C}{2} + \left(1 + \frac{ik_2}{k_1}\right)\frac{D}{2} \tag{7}$$

$$B = \left(1 + \frac{ik_2}{k_1}\right)\frac{C}{2} + \left(1 - \frac{ik_2}{k_1}\right)\frac{D}{2} \tag{8}$$

Substituting (5) and (6) into (7) and solving for the transmission amplitude F/A, we find the transmission probability $T = \left|\frac{F}{A}\right|^2$. This yields the well-known analytical result:

$$T = \frac{1}{\cosh^2(k_2 L) + \frac{\gamma^2}{4}\sinh^2(k_2 L)}$$

where $\gamma = \frac{k_1^2 - k_2^2}{k_1 k_2}$.

Method 2: Transfer Matrix Approach

We can rewrite the equations from the boundary conditions in matrix form. The transfer matrix operator $\hat{O}$ relates the coefficients in Region I to the final coefficients in Region III

$$\begin{pmatrix} A \\ B \end{pmatrix} = \hat{O}\begin{pmatrix} F \\ 0 \end{pmatrix}$$

The operator $\hat{O}$ is a product of three operators: $\hat{O} = \hat{M}_\alpha \cdot \hat{M}_\beta \cdot \hat{M}_\eta$.

- **Operator $\hat{M}_\alpha$ (Interface at $x = 0$):** From equations (7) and (8), we relate (A, B) to (C, D):

$$\begin{pmatrix} A \\ B \end{pmatrix} = \hat{M}_\alpha \begin{pmatrix} C \\ D \end{pmatrix} \quad \text{where} \quad \hat{M}_\alpha = \frac{1}{2}\begin{pmatrix} 1 - \frac{ik_2}{k_1} & 1 + \frac{ik_2}{k_1} \\ 1 + \frac{ik_2}{k_1} & 1 - \frac{ik_2}{k_1} \end{pmatrix}$$

- **Propagation Operator $\hat{M}_\beta$:** This operator propagates the wave function through Region II, from $x = 0$ to $x = L$. Let $C' = Ce^{k_2 L}$ and $D' = De^{-k_2 L}$ be the amplitudes at $x = L$. We relate $\begin{pmatrix} C \\ D \end{pmatrix}$ to $\begin{pmatrix} C' \\ D' \end{pmatrix}$:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \hat{M}_\beta \begin{pmatrix} C' \\ D' \end{pmatrix} \quad \text{where} \quad \hat{M}_\beta = \begin{pmatrix} e^{-k_2 L} & 0 \\ 0 & e^{k_2 L} \end{pmatrix}$$

- **Operator $\hat{M}_\eta$ (Interface at $x = L$):** This operator relates the amplitudes in Region II at $x = L$ (C', D') to the amplitudes in Region III at $x = L$. $\psi_{III}(x) = Fe^{ik_1 x}$. At $x = L$, the amplitudes are $Fe^{ik_1 L}$.

$$\begin{pmatrix} C' \\ D' \end{pmatrix} = \hat{M}_\eta \begin{pmatrix} Fe^{ik_1 L} \\ 0 \end{pmatrix}$$

  From solving equations (2) and (4), this boundary operator is:

$$\hat{M}_\eta = \frac{1}{2} \begin{pmatrix} 1 + \frac{ik_1}{k_2} & 1 - \frac{ik_1}{k_2} \\ 1 - \frac{ik_1}{k_2} & 1 + \frac{ik_1}{k_2} \end{pmatrix}$$

The total relationship is:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \left(\hat{M}_\alpha \hat{M}_\beta \hat{M}_\eta \right) \begin{pmatrix} Fe^{ik_1 L} \\ 0 \end{pmatrix}$$

Let $\hat{O} = \hat{M}_\alpha \hat{M}_\beta \hat{M}_\eta$. We only need the O_{11} element:

$$A = O_{11}(Fe^{ik_1 L})$$

Operator $\hat{O}$ Elements

$$O_{11} = (M_{\alpha,11})(M_{\beta,11})(M_{\eta,11}) + (M_{\alpha,12})(M_{\beta,22})(M_{\eta,21})$$

$$O_{11} = \left[\frac{1}{2} \left(1 - \frac{ik_2}{k_1} \right) \right] \left[e^{-k_2 L} \right] \left[\frac{1}{2} \left(1 + \frac{ik_1}{k_2} \right) \right] + \left[\frac{1}{2} \left(1 + \frac{ik_2}{k_1} \right) \right] \left[e^{k_2 L} \right] \left[\frac{1}{2} \left(1 - \frac{ik_1}{k_2} \right) \right]$$

$$O_{11} = \frac{1}{4} \left[\left(1 - \frac{ik_2}{k_1} \right) \left(1 + \frac{ik_1}{k_2} \right) e^{-k_2 L} + \left(1 + \frac{ik_2}{k_1} \right) \left(1 - \frac{ik_1}{k_2} \right) e^{k_2 L} \right]$$

where $\gamma = \frac{k_1^2 - k_2^2}{k_1 k_2}$:

- $\left(1 - \frac{ik_2}{k_1} \right) \left(1 + \frac{ik_1}{k_2} \right) = 2 + i\gamma$
- $\left(1 + \frac{ik_2}{k_1} \right) \left(1 - \frac{ik_1}{k_2} \right) = 2 - i\gamma$

We get:

$$O_{11} = \frac{1}{4}\left[(2+i\gamma)e^{-k_2 L} + (2-i\gamma)e^{k_2 L}\right]$$

$$\begin{aligned}
O_{11} &= \frac{1}{4}\left[2(e^{k_2 L} + e^{-k_2 L}) - i\gamma(e^{k_2 L} - e^{-k_2 L})\right] \\
&= \frac{1}{4}\left[4\cosh(k_2 L) - 2i\gamma\sinh(k_2 L)\right] \\
&= \cosh(k_2 L) - \frac{i\gamma}{2}\sinh(k_2 L)
\end{aligned}$$

Conclusion: Equivalence

From $A = O_{11}(Fe^{ik_1 L})$, the transmission amplitude is

$$\frac{F}{A} = \frac{1}{O_{11}e^{ik_1 L}} = \frac{e^{-ik_1 L}}{O_{11}}$$

$$\frac{F}{A} = \frac{e^{-ik_1 L}}{\cosh(k_2 L) - \frac{i\gamma}{2}\sinh(k_2 L)}$$

This exactly matches the analytical result derived earlier. Calculating the transmission probability $T = \left|\frac{F}{A}\right|^2$:

$$T = \left|\frac{e^{-ik_1 L}}{\cosh(k_2 L) - \frac{i\gamma}{2}\sinh(k_2 L)}\right|^2 = \frac{|e^{-ik_1 L}|^2}{\left|\cosh(k_2 L) - \frac{i\gamma}{2}\sinh(k_2 L)\right|^2}$$

$$T = \frac{1}{\cosh^2(k_2 L) + \frac{\gamma^2}{4}\sinh^2(k_2 L)}$$

This demonstrates that the standard Transfer Matrix method and the standard Analytical Solution are equivalent, yielding the identical result.