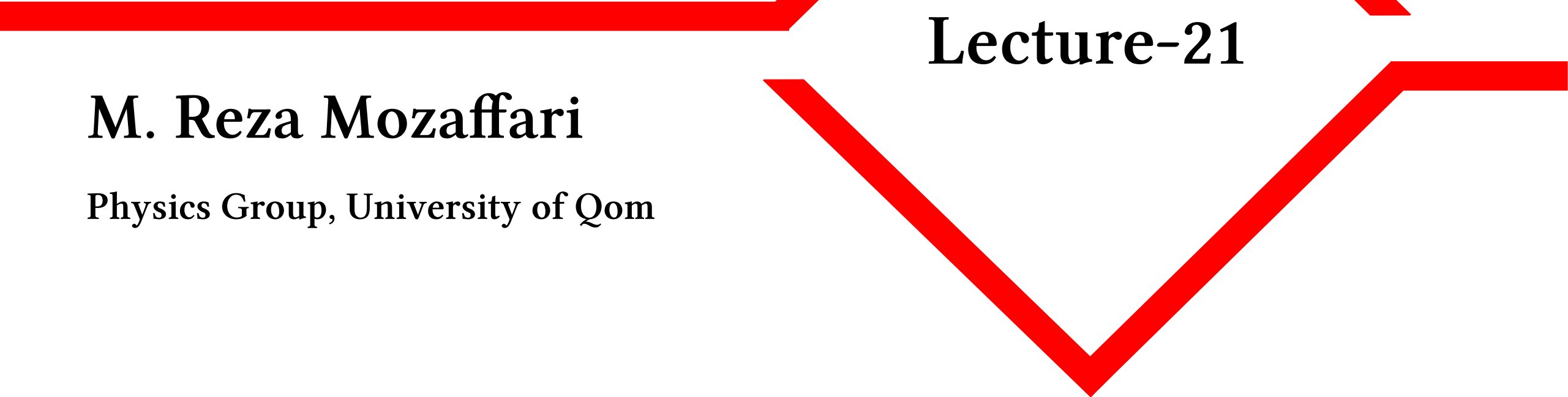


# Computational Physics



## Lecture-19

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# Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root
- Classical Scattering
- Solving Linear Systems
- Transmission of Rectangular Barriers

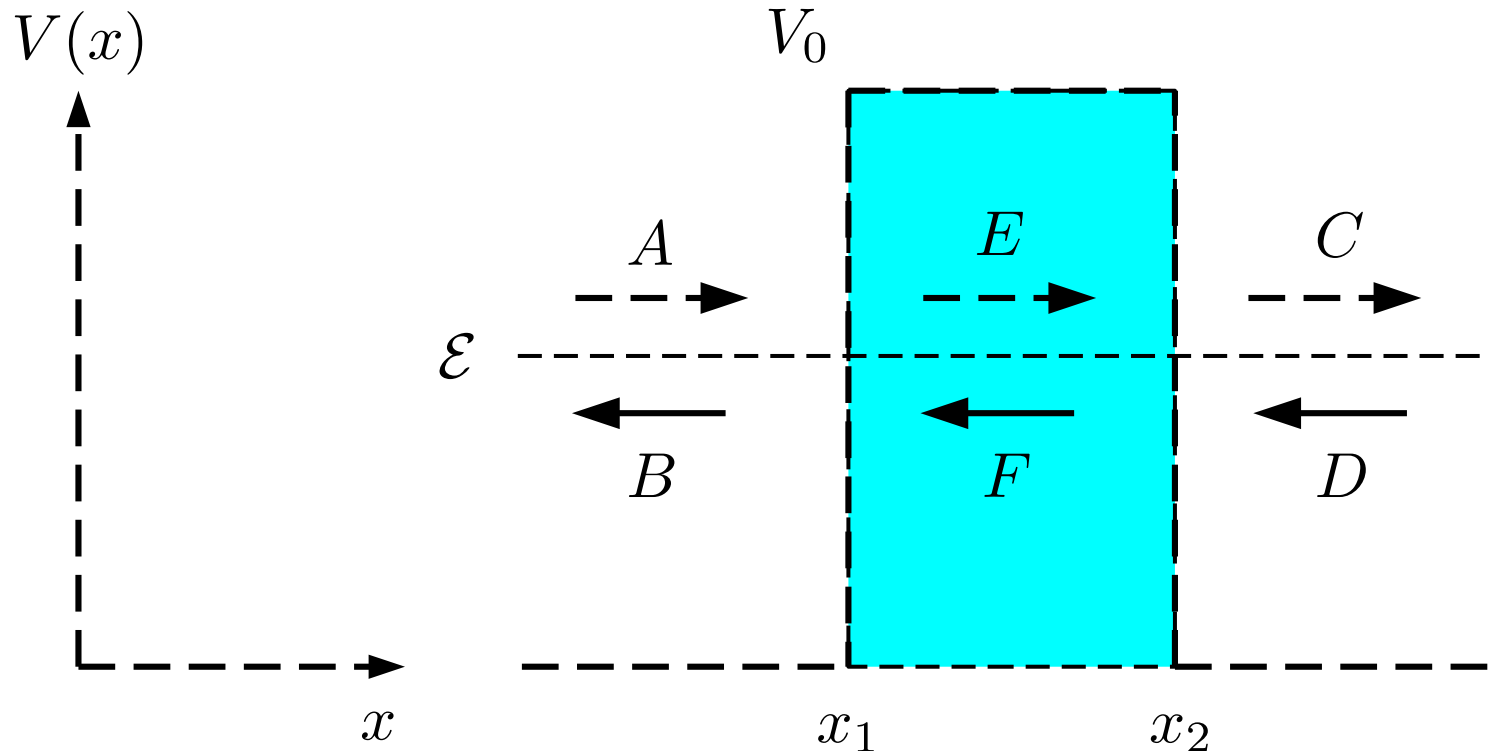
# Transmission of Rectangular Barriers

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

$$\left\{ \begin{array}{l} -\frac{\hbar^2}{2m} \frac{d^2\psi_{\text{I}}}{dx^2} = \mathcal{E}\psi_{\text{I}} \\ -\frac{\hbar^2}{2m} \frac{d^2\psi_{\text{II}}}{dx^2} + V_0\psi_{\text{II}} = \mathcal{E}\psi_{\text{II}} \\ -\frac{\hbar^2}{2m} \frac{d^2\psi_{\text{III}}}{dx^2} = \mathcal{E}\psi_{\text{III}} \end{array} \right.$$

$$\left\{ \begin{array}{l} \psi_{\text{I}} = Ae^{ikx} + Be^{-ikx} \\ \psi_{\text{II}} = Ee^{qx} + Fe^{-qx} \\ \psi_{\text{III}} = Ce^{ikx} + De^{-ikx} \end{array} \right.$$

$$k = \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}, \quad q = \sqrt{\frac{2m(V_0 - \mathcal{E})}{\hbar^2}}$$



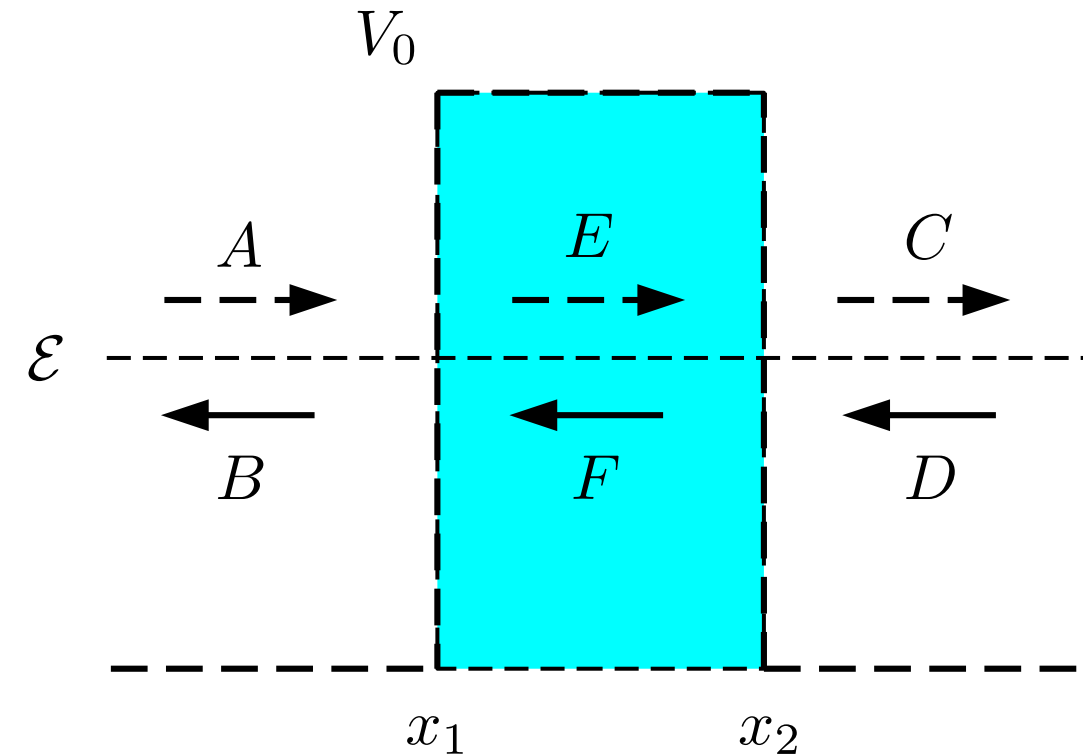
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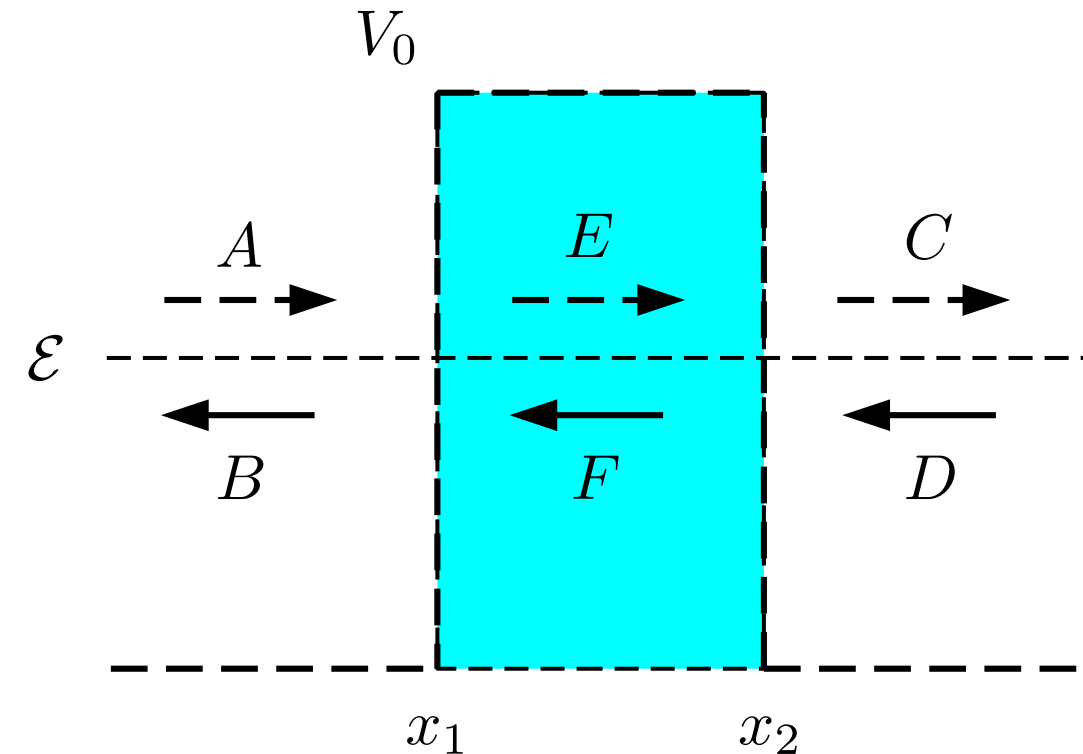


# Transmission of Rect...

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

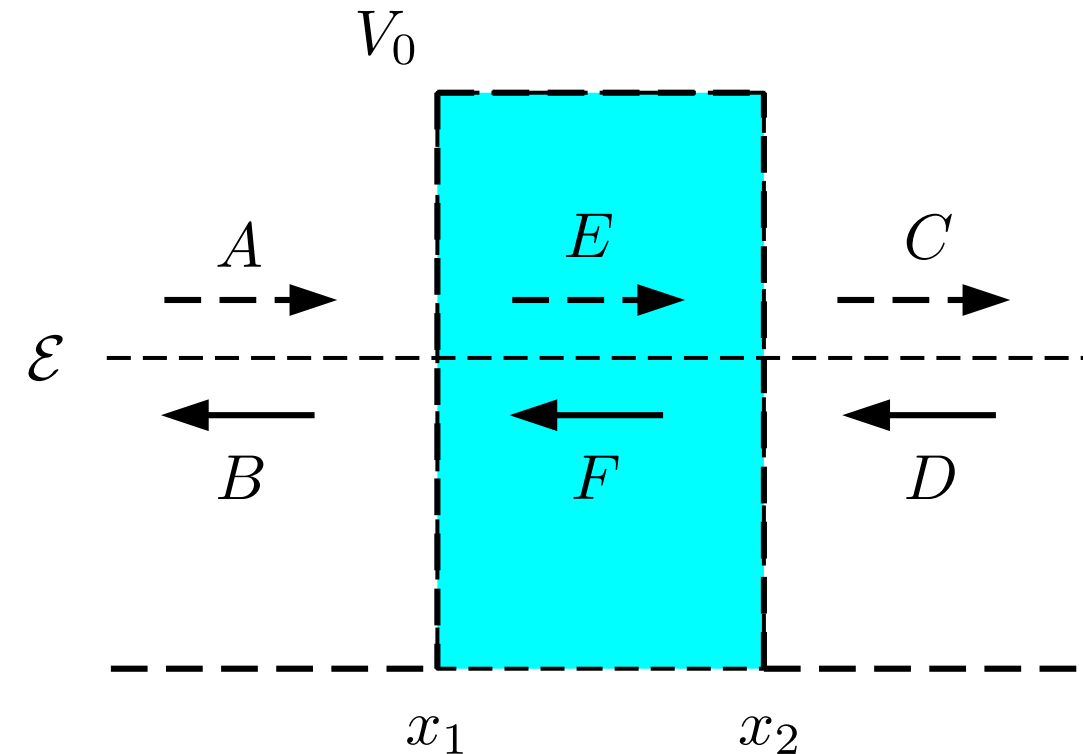
$$\left\{ \begin{array}{l} Ae^{ikx_1} + Be^{-ikx_1} = Ee^{qx_1} + Fe^{-qx_1} \\ ik(Ae^{ikx_1} - Be^{-ikx_1}) = q(Ee^{qx_1} - Fe^{-qx_1}) \\ Ee^{qx_2} + Fe^{-qx_2} = Ce^{ikx_2} + De^{-ikx_2} \\ q(Ee^{qx_2} - Fe^{-qx_2}) = ik(Ce^{ikx_2} - De^{-ikx_2}) \end{array} \right.$$

$$\left[ \begin{array}{cc} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{array} \right] \left[ \begin{array}{c} A \\ B \end{array} \right] = \left[ \begin{array}{cc} e^{qx_1} & e^{-qx_1} \\ qe^{qx_1} & -qe^{-qx_1} \end{array} \right] \left[ \begin{array}{c} E \\ F \end{array} \right]$$



# Transmission of Rect...

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



$$\left\{ \begin{array}{l} Ae^{ikx_1} + Be^{-ikx_1} = Ee^{qx_1} + Fe^{-qx_1} \\ ik(Ae^{ikx_1} - Be^{-ikx_1}) = q(Ee^{qx_1} - Fe^{-qx_1}) \\ \hline Ee^{qx_2} + Fe^{-qx_2} = Ce^{ikx_2} + De^{-ikx_2} \\ q(Ee^{qx_2} - Fe^{-qx_2}) = ik(Ce^{ikx_2} - De^{-ikx_2}) \end{array} \right.$$

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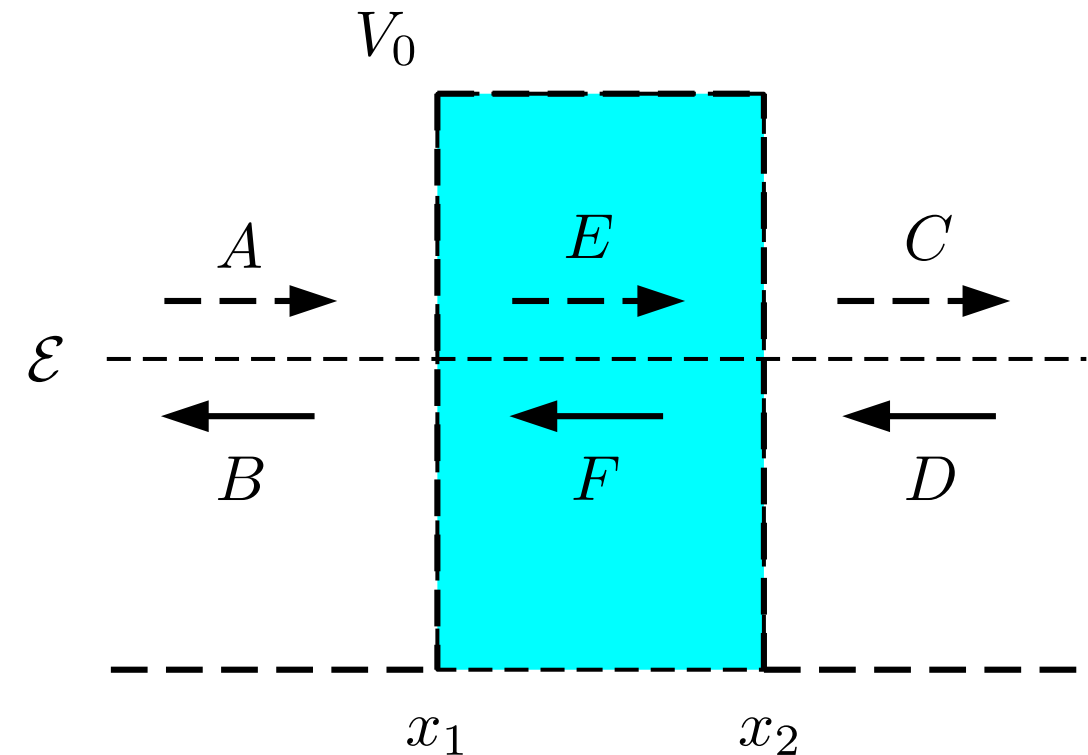
$$\begin{bmatrix} e^{qx_1} & e^{-qx_1} \\ qe^{qx_1} & -qe^{-qx_1} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}$$

$$\begin{bmatrix} e^{qx_2} & e^{-qx_2} \\ qe^{qx_2} & -qe^{-qx_2} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} =$$

$$\begin{bmatrix} e^{ikx_2} & e^{-ikx_2} \\ ike^{ikx_2} & -ike^{-ikx_2} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}$$

# Transmission of Rectangular Barriers

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



$$M_1 = \begin{bmatrix} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{bmatrix}$$

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$$M_1 \begin{bmatrix} A \\ B \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

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# Transmission of Rectangular Barriers

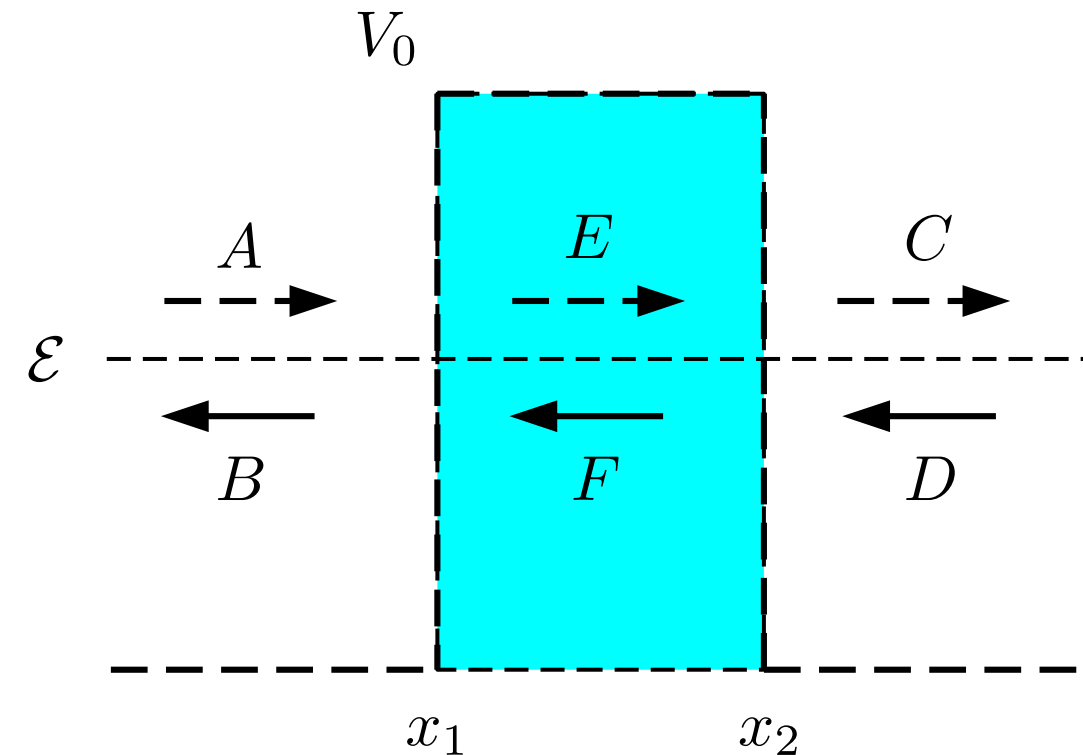
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = \mathcal{E}\psi$$

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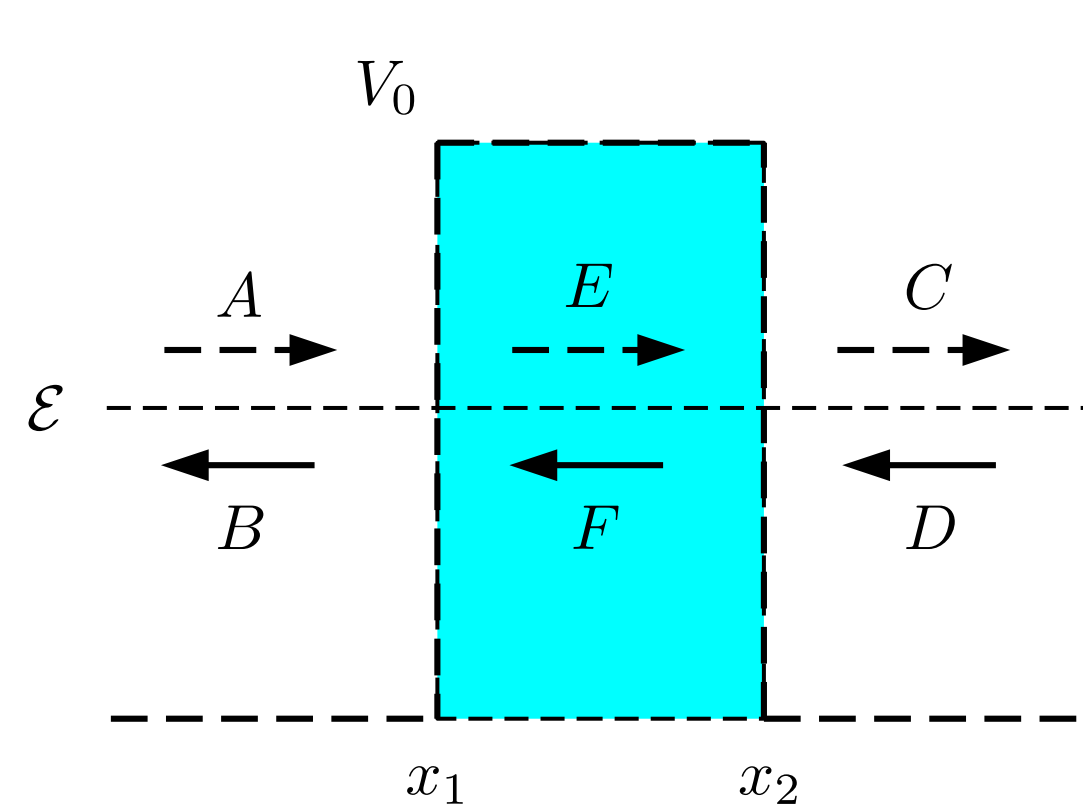


# Transmission of Rectangular Barriers

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

$$M_1 \begin{bmatrix} A \\ B \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

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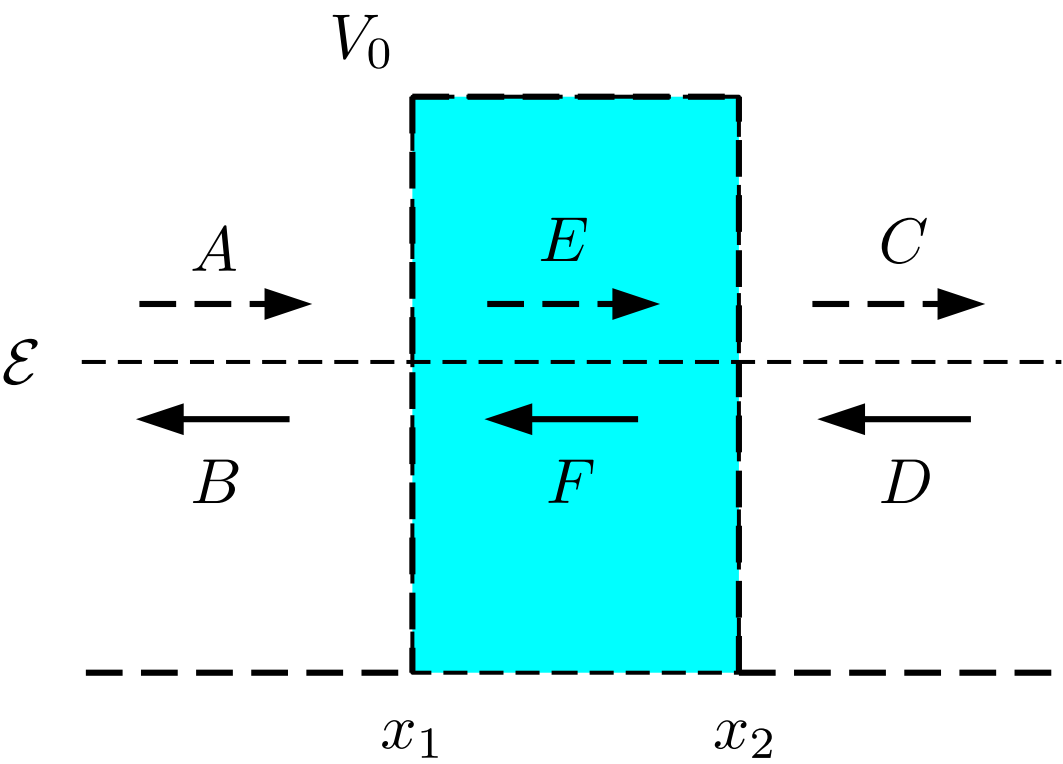
$$M_4^{-1} M_3 \begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

$$M_4^{-1} M_3 M_2^{-1} M_1 \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\mathcal{M} = M_4^{-1} M_3 M_2^{-1} M_1, \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}$$

# Transmission of Rectangular Barriers

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



$$M_1 = \begin{bmatrix} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{bmatrix}$$

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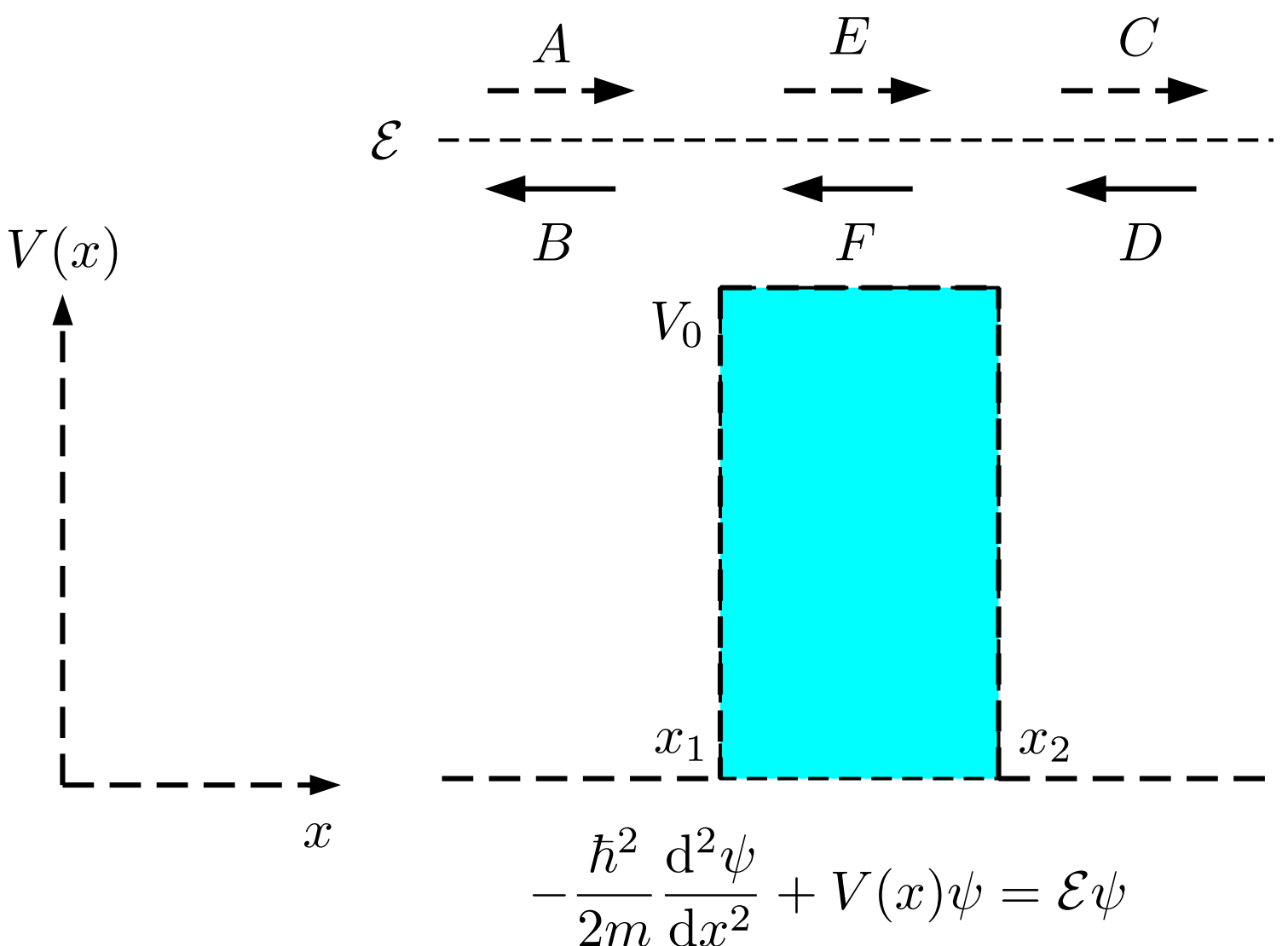
$$M_4 = \begin{bmatrix} e^{ikx_2} & e^{-ikx_2} \\ ike^{ikx_2} & -ike^{-ikx_2} \end{bmatrix}$$

$$\mathcal{M} = M_4^{-1} M_3 M_2^{-1} M_1, \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}$$

$$\mathcal{M} = \mathcal{M}(V_0, \mathcal{E}, x_1, x_2)$$

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# Transmission of Rectangular Barriers

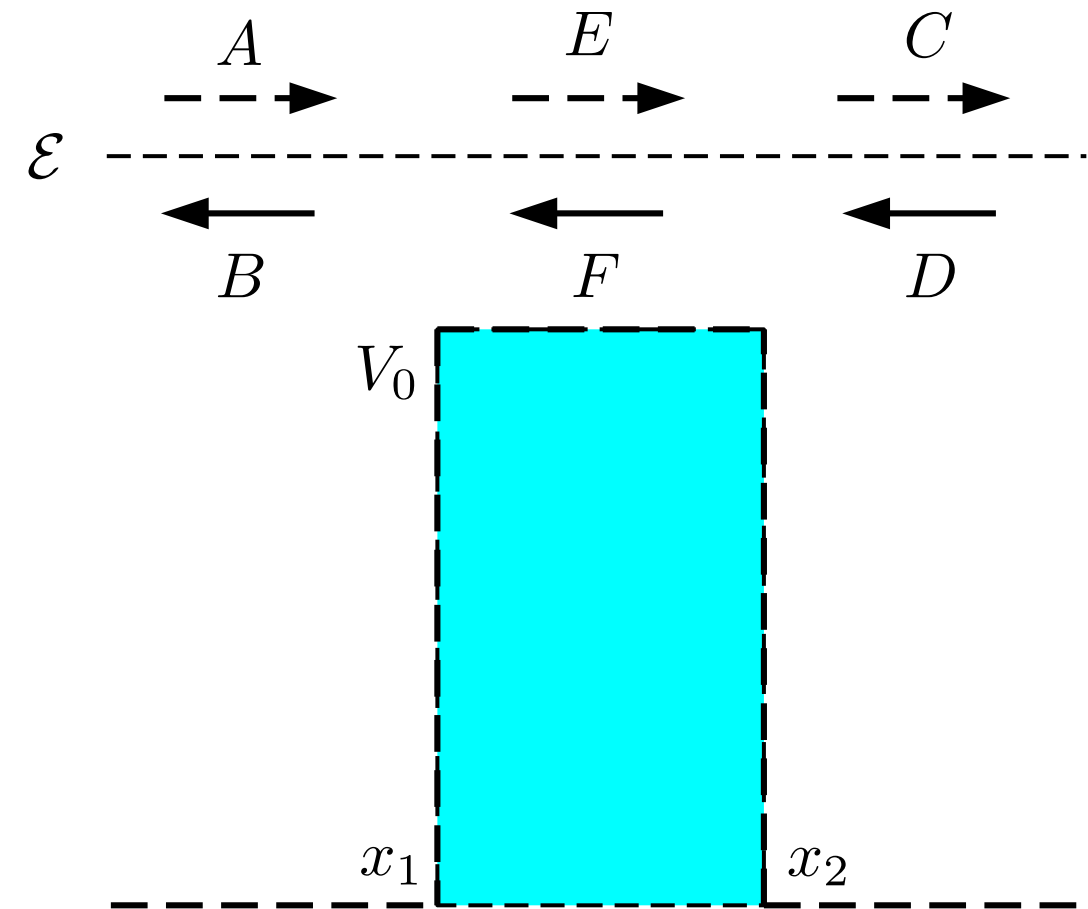


$$\left\{ \begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi_{\text{I}}}{dx^2} &= \mathcal{E}\psi_{\text{I}} \\ -\frac{\hbar^2}{2m} \frac{d^2\psi_{\text{II}}}{dx^2} + V_0\psi_{\text{II}} &= \mathcal{E}\psi_{\text{II}} \\ -\frac{\hbar^2}{2m} \frac{d^2\psi_{\text{III}}}{dx^2} &= \mathcal{E}\psi_{\text{III}} \end{aligned} \right.$$

$$\left\{ \begin{aligned} \psi_{\text{I}} &= Ae^{ikx} + Be^{-ikx} \\ \psi_{\text{II}} &= Ee^{iqx} + Fe^{-iqx} \\ \psi_{\text{III}} &= Ce^{ikx} + De^{-ikx} \end{aligned} \right.$$

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# Transmission of Rectangular Barriers



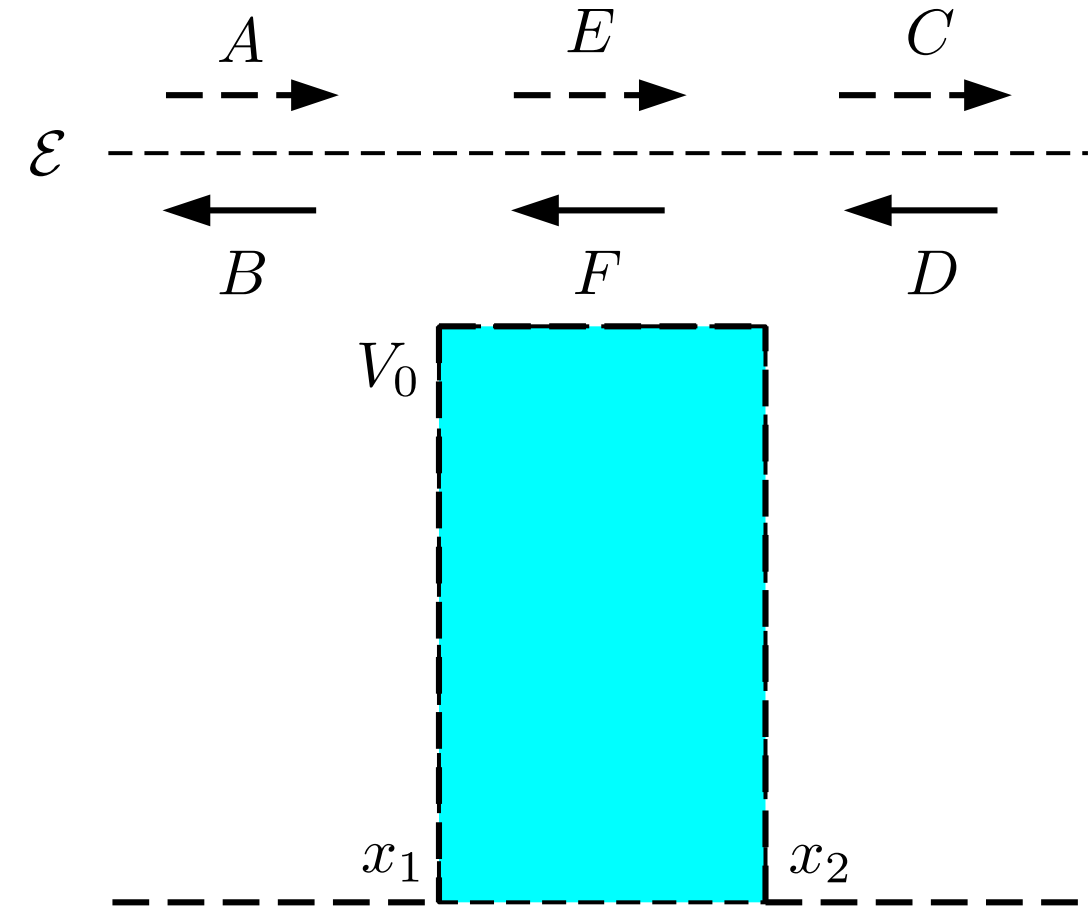
$$\begin{cases} \psi_{\text{I}} = Ae^{ikx} + Be^{-ikx} \\ \psi_{\text{II}} = Ee^{iqx} + Fe^{-iqx} \\ \psi_{\text{III}} = Ce^{ikx} + De^{-ikx} \end{cases}$$

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

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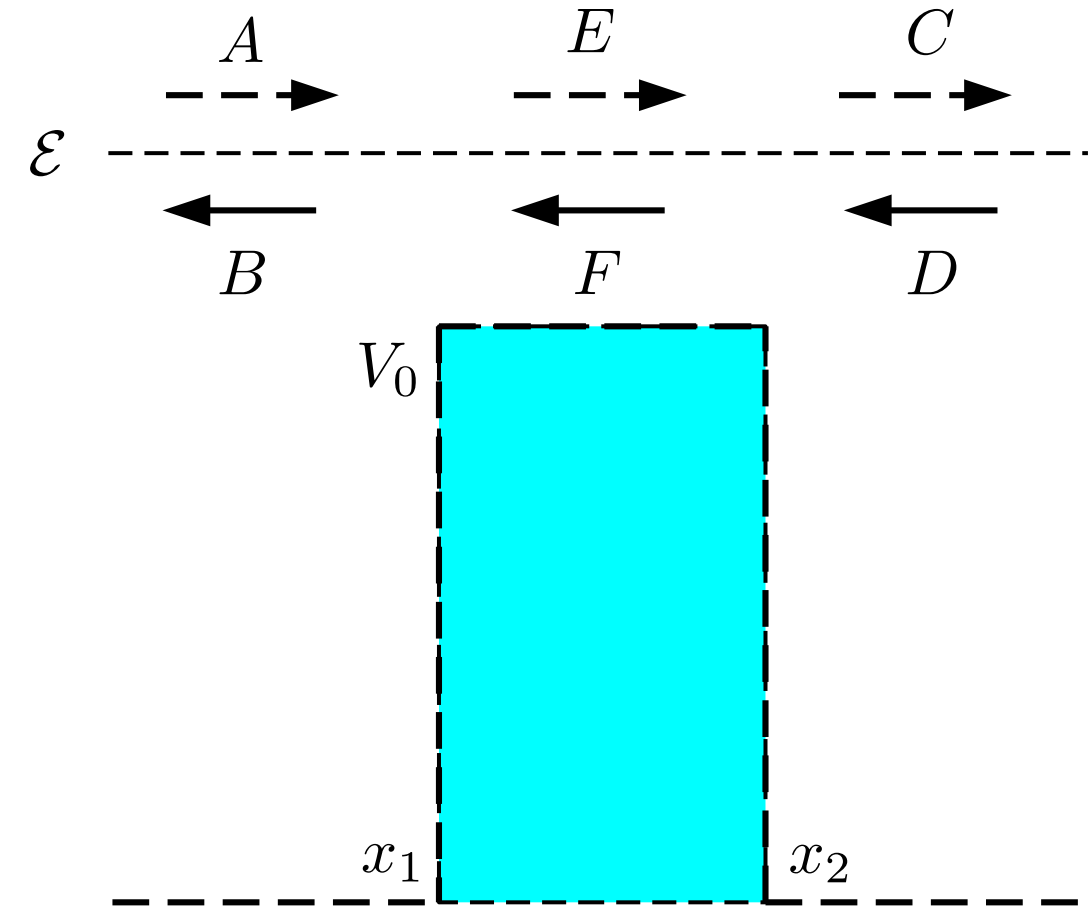


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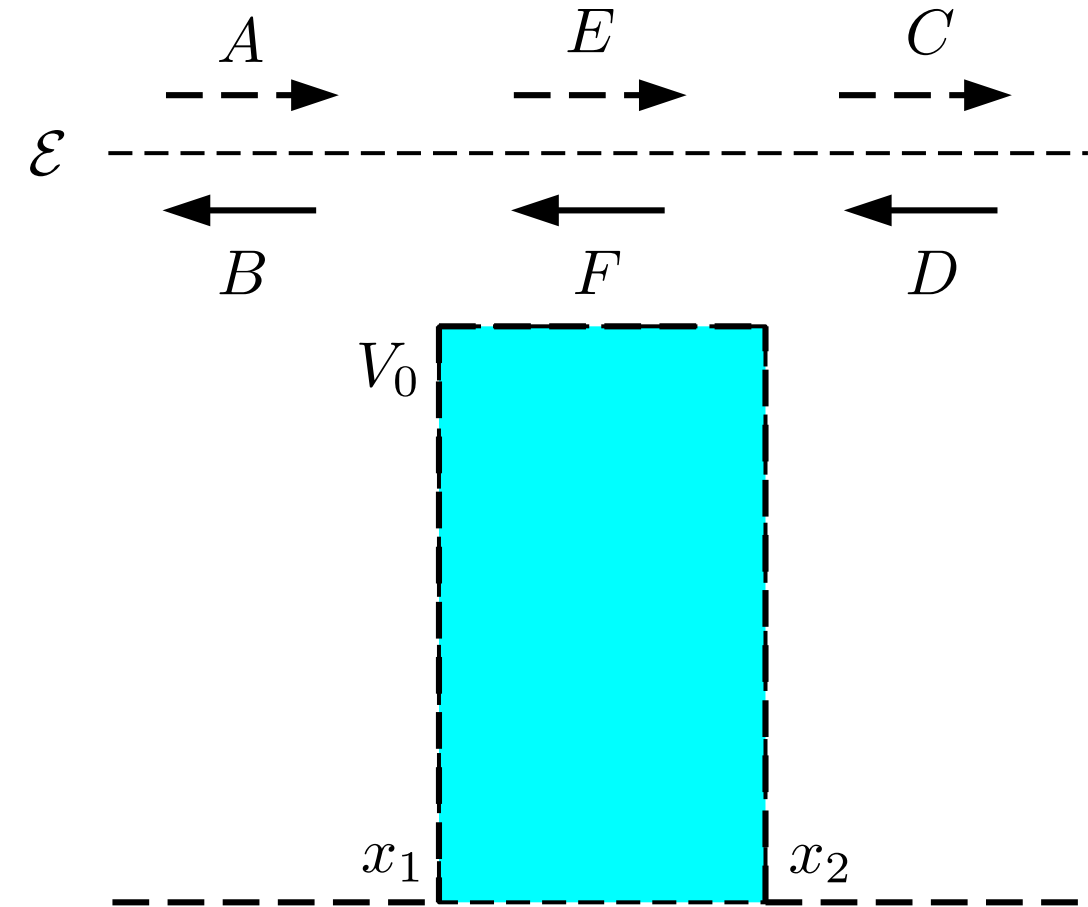
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# Transmission of Rectangular Barriers



$$M_1 = \begin{bmatrix} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{bmatrix}$$

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

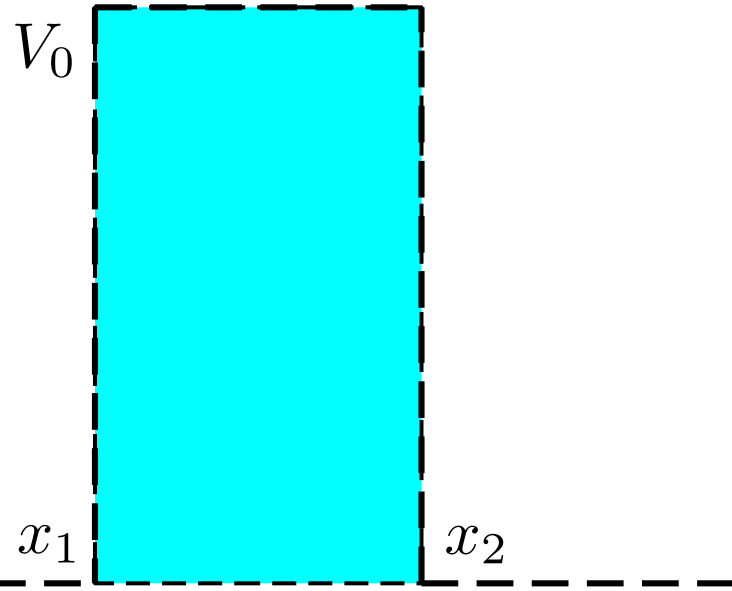
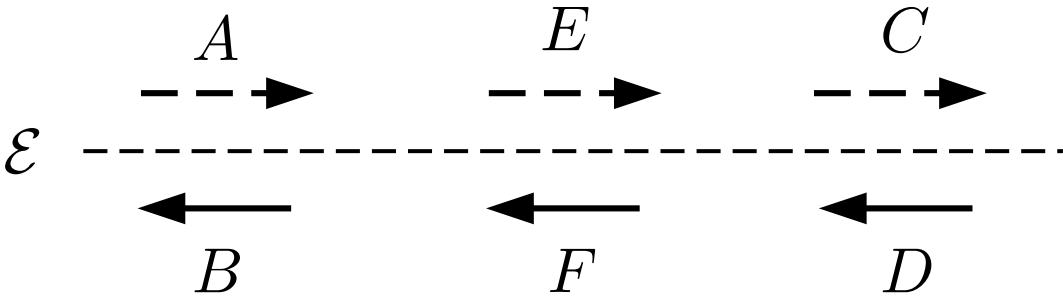
# Transmission of Rectangular Barriers

$$M_1 \begin{bmatrix} A \\ B \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

$$M_3 \begin{bmatrix} E \\ F \end{bmatrix} = M_4 \begin{bmatrix} C \\ D \end{bmatrix}$$

$$M_2^{-1} M_1 \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} E \\ F \end{bmatrix}$$

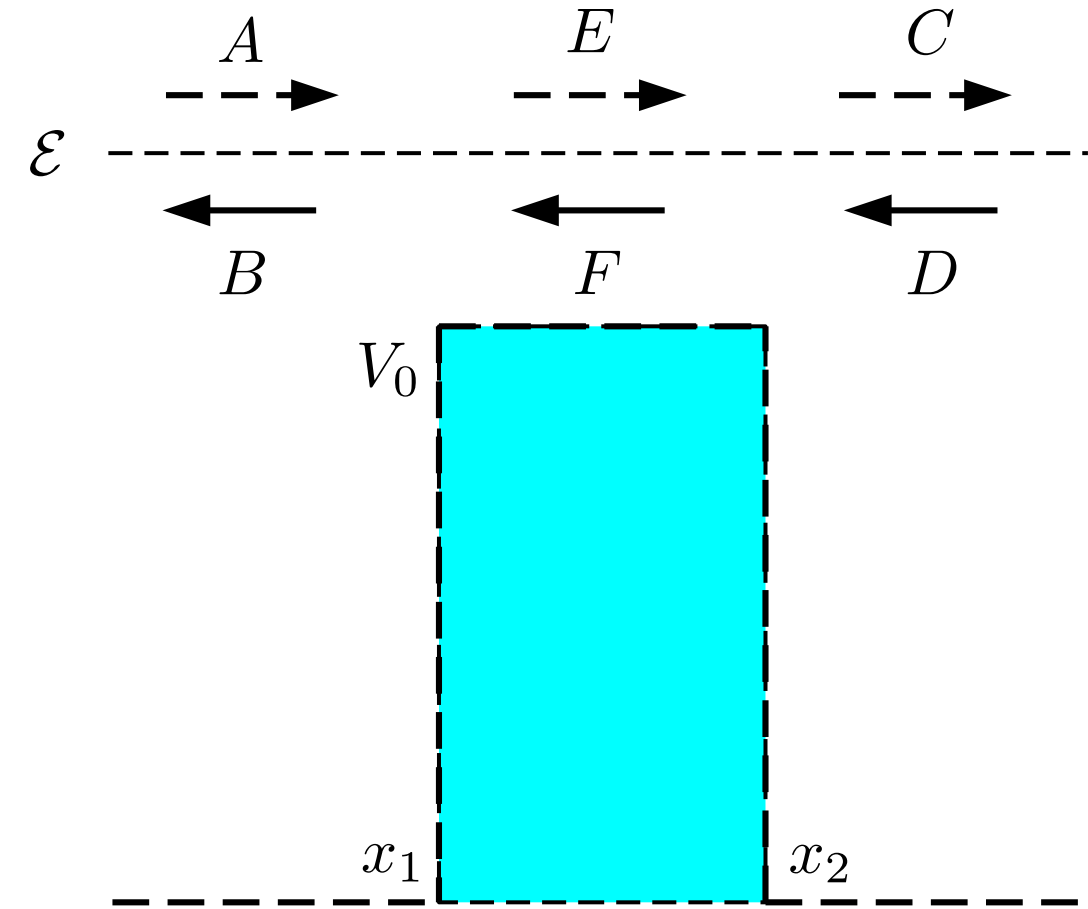
$$M_4^{-1} M_3 \begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$



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



# Transmission of Rectangular Barriers



$$M_1 \begin{bmatrix} A \\ B \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

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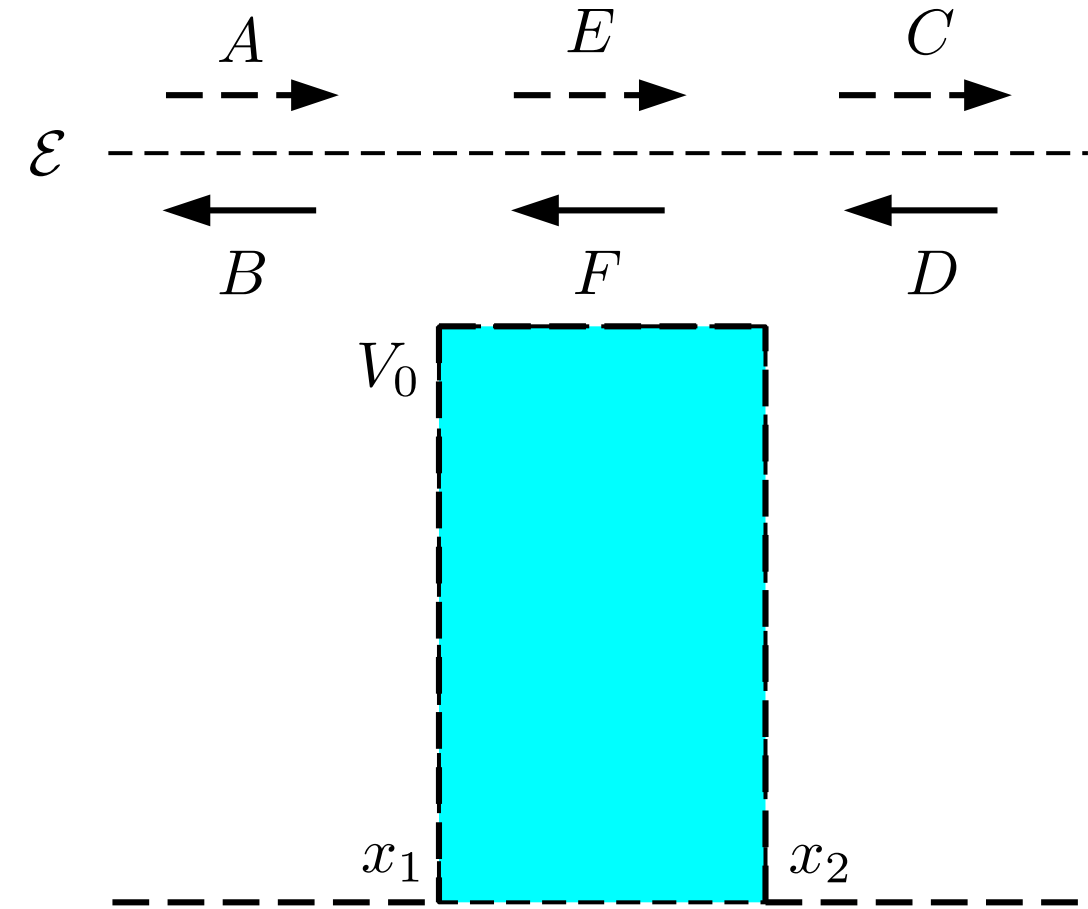
$$M_4^{-1} M_3 \begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

$$M_4^{-1} M_3 M_2^{-1} M_1 \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

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

$$\mathcal{M} = M_4^{-1} M_3 M_2^{-1} M_1, \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}$$

# Transmission of Rectangular Barriers



$$M_1 = \begin{bmatrix} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{bmatrix}$$

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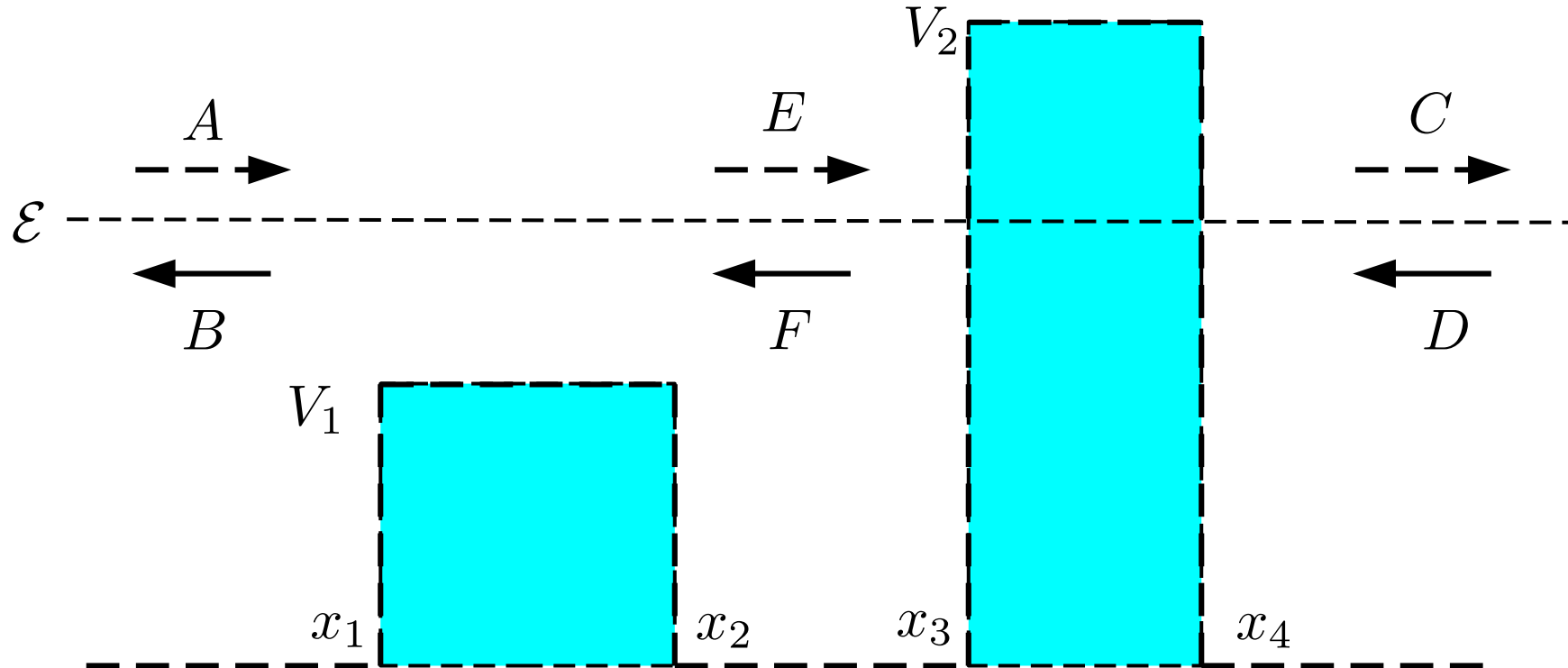
$$\mathcal{M} = M_4^{-1} M_3 M_2^{-1} M_1, \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}$$

$$\mathcal{M} = \mathcal{M}(V_0, \mathcal{E}, x_1, x_2)$$

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

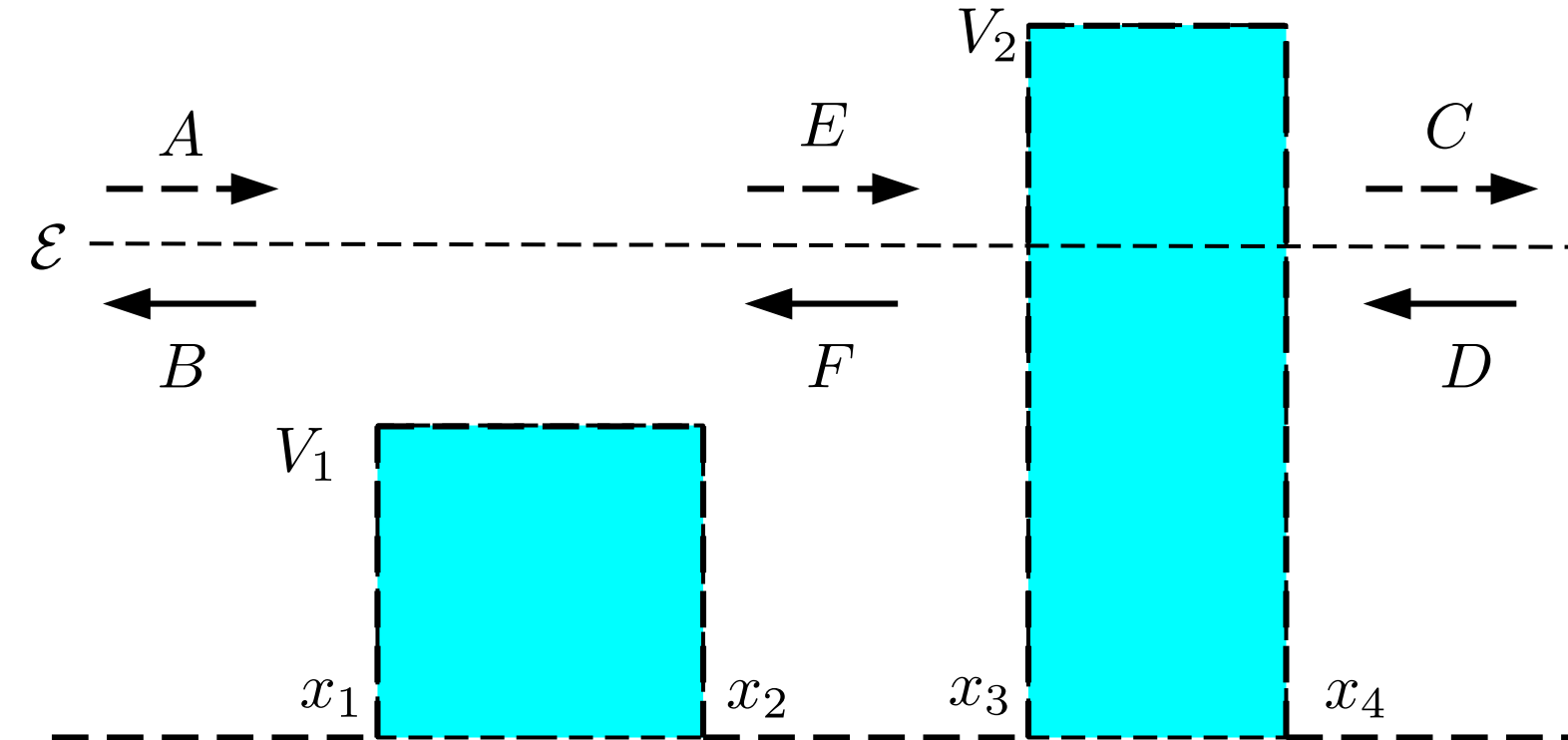
$$k = \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}, \quad q = \sqrt{\frac{2m(\mathcal{E} - V_0)}{\hbar^2}}$$

# Transmission of Rectangular Barriers



$$\begin{bmatrix} E \\ F \end{bmatrix} = \mathcal{M}_1 \begin{bmatrix} A \\ B \end{bmatrix} \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M}_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

# Transmission of Rectangular Barriers



$$\mathcal{M}_1 = \mathcal{M}_1(V_1, \mathcal{E}, x_1, x_2)$$

$$k = \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}, \quad q = \sqrt{\frac{2m(\mathcal{E} - V_1)}{\hbar^2}}$$

$$\mathcal{M}_2 = \mathcal{M}_2(V_2, \mathcal{E}, x_3, x_4)$$

$$k = \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}, \quad q = \sqrt{\frac{2m(V_2 - \mathcal{E})}{\hbar^2}}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M}_2 \mathcal{M}_1 \begin{bmatrix} A \\ B \end{bmatrix}$$

$$\begin{bmatrix} E \\ F \end{bmatrix} = \mathcal{M}_1 \begin{bmatrix} A \\ B \end{bmatrix} \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M}_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

$$\mathcal{M} = \mathcal{M}_2 \mathcal{M}_1, \quad \begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}$$

# Transmission of Rectangular Barriers

$$\begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}, \quad D = 0$$

$$\begin{bmatrix} C \\ 0 \end{bmatrix} = \begin{bmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathcal{M}_{22} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}$$

$$\mathcal{M}_{21}A + \mathcal{M}_{22}B = 0 \Rightarrow \frac{B}{A} = -\frac{\mathcal{M}_{21}}{\mathcal{M}_{22}}$$

$$C = \mathcal{M}_{11}A + \mathcal{M}_{12}B \Rightarrow \frac{C}{A} = \mathcal{M}_{11} + \mathcal{M}_{12}\frac{B}{A}$$

$$r = \frac{B}{A} = -\frac{\mathcal{M}_{21}}{\mathcal{M}_{22}}$$

$$t = \frac{C}{A} = \mathcal{M}_{11} - \mathcal{M}_{12}\frac{\mathcal{M}_{21}}{\mathcal{M}_{22}}$$

$$R = |r|^2 = rr^* = \left| \frac{\mathcal{M}_{21}}{\mathcal{M}_{22}} \right|^2$$

$$T = |t|^2 = tt^* = \left| \mathcal{M}_{11} - \mathcal{M}_{12}\frac{\mathcal{M}_{21}}{\mathcal{M}_{22}} \right|^2$$

# Transmission of Rectangular Barriers

$$\begin{bmatrix} C \\ D \end{bmatrix} = \mathcal{M} \begin{bmatrix} A \\ B \end{bmatrix}, \quad D = 0$$

$$\begin{bmatrix} C \\ 0 \end{bmatrix} = \begin{bmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathcal{M}_{22} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}$$

$$r = \frac{B}{A} = -\frac{\mathcal{M}_{21}}{\mathcal{M}_{22}}$$

$$t = \frac{C}{A} = \mathcal{M}_{11} - \mathcal{M}_{12} \frac{\mathcal{M}_{21}}{\mathcal{M}_{22}}$$

$$R = |r|^2 = rr^* = \left| \frac{\mathcal{M}_{21}}{\mathcal{M}_{22}} \right|^2$$

$$T = |t|^2 = tt^* = \left| \mathcal{M}_{11} - \mathcal{M}_{12} \frac{\mathcal{M}_{21}}{\mathcal{M}_{22}} \right|^2$$

$$T(\mathcal{E}) + R(\mathcal{E}) = 1$$

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