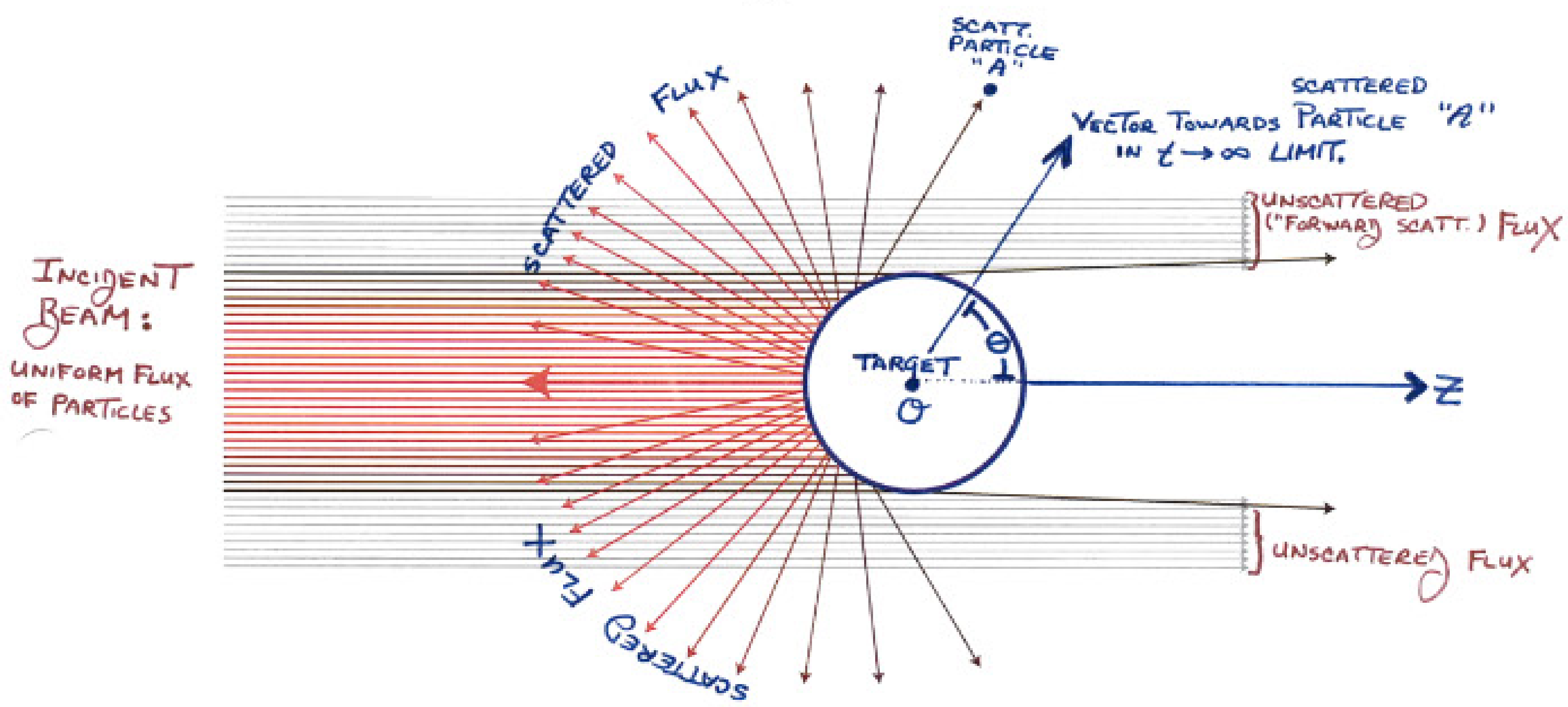
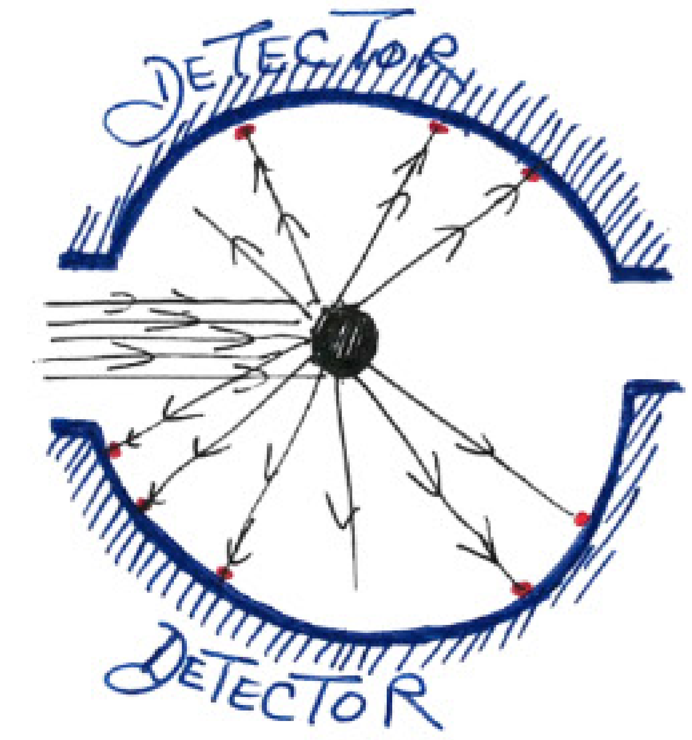
Quantum Scattering Theory: 1D Version

- Send a "beam" of particles at a target (e.g. e^-'s flung into a nucleus)
- Measure scattered flux of particles



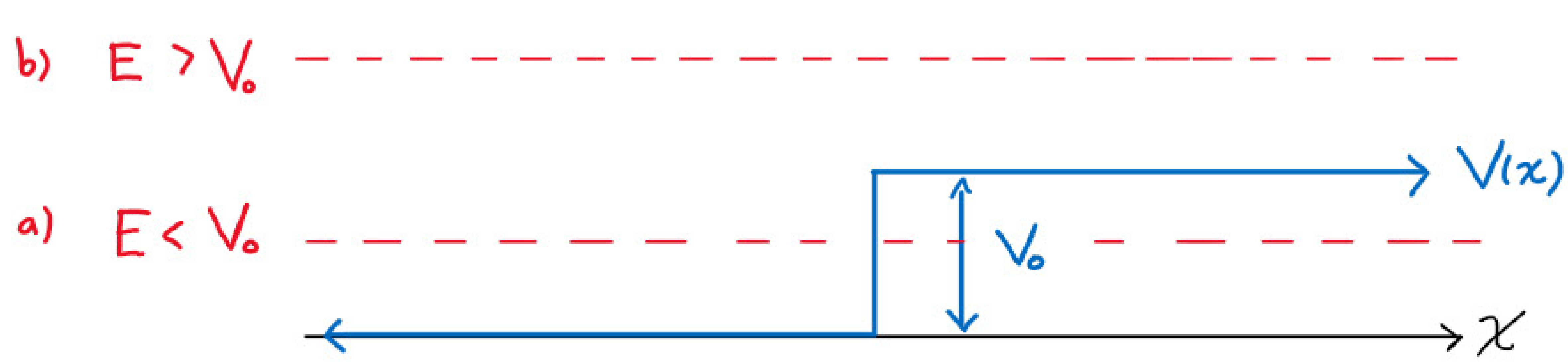


- Many physics experiments work this way
  - Large Hadron Collider at CERN (High energy particle, Nuclear Physics)
  - Neutron Scattering
  - Photo Emission Spectroscopy (Condensed Matter / Materials Physics)
- Both target and projectile are Quantum Mechanical!

Simplest Version: Quantum Scattering off a Potential in 1D

- Directly relevant to conduction in "single channel" quantum wires, i.e.
  - SW Carbon NanoTubes
  - Edge states of 2D Topological Insulators

① Step Barrier



$$\hat{H}|E\rangle = E|E\rangle \implies -\frac{d^2}{dx^2}\psi_E(x) = \left(\frac{2m}{\hbar^2}\right)[E - V(x)]\,\psi_E(x) \quad ; \quad \psi_{E(x)} \equiv \begin{cases} \psi_<(x), & x<0 \\ \psi_>(x), & x \geq 0 \end{cases}$$

a) $0 \leq E < V_0$: TUNNELING (EXP. DECAY) INTO THE STEP.

$$\psi_<(x) = A\,e^{iK_1 x} + B\,e^{-iK_1 x} \quad ; \quad K_1 = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} \geq 0 \text{ W.L.O.G.}$$

$$\psi_>(x) = C\,e^{-K_2 x} + \cancel{D\,e^{K_2 x}} \quad ; \quad K_2 = \left[\frac{2m}{\hbar^2}\left(V_0 - E\right)\right]^{1/2} \geq 0 \text{ FOR } 0 \leq E \leq V_0.$$

NOT PHYSICALLY SENSIBLE

CONTINUITY CONDITIONS: $-\psi''_E(x) = \frac{2m}{\hbar^2}[E - V_0(x)]\psi_E(x) \implies \psi''_E$ HAS A FINITE DISCONTINUITY @ $x=0$

$\therefore$ ψ'_E AND ψ_E ARE CONTINUOUS THERE.

① $\psi_< = \psi_>$: $A + B = C$

② $\psi'_< = \psi'_>$: $iK_1(A-B) = -K_2 C$

$\implies$ $2iK_1 A = (iK_1 - K_2)C$

$K_2 A + K_2 B + iK_1 A - iK_1 B = 0$

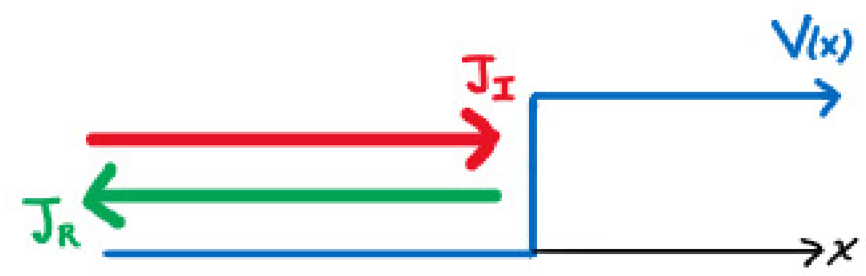
$$\boxed{C = \frac{2iK_1}{iK_1 - K_2}A \qquad B = \frac{iK_1 + K_2}{iK_1 - K_2}A}$$

PROBABILITY CURRENTS $\quad J = \frac{\hbar}{m}\,\mathrm{Im}\left[\psi^* \frac{d}{dx}\psi\right]$

$x<0$: $\psi^*\frac{d}{dx}\psi = iK_1\left[A^* e^{-iK_1 x} + B^* e^{iK_1 x}\right]\left[A e^{iK_1 x} - B e^{-iK_1 x}\right] = iK_1\left[|A|^2 - |B|^2 + \underbrace{\left(B^* A e^{2iK_1 x} - c.c.\right)}_{\text{PURE IMAGINARY}}\right]$

$\therefore$ $J_<(x) = \frac{\hbar K_1}{m}\left[|A|^2 - |B|^2\right] \equiv J_I - J_R$, "INCIDENT" FLUX $J_I \equiv \frac{\hbar K_1}{m}|A|^2$

"REFLECTED" FLUX $J_R \equiv \frac{\hbar K_1}{m}|B|^2$

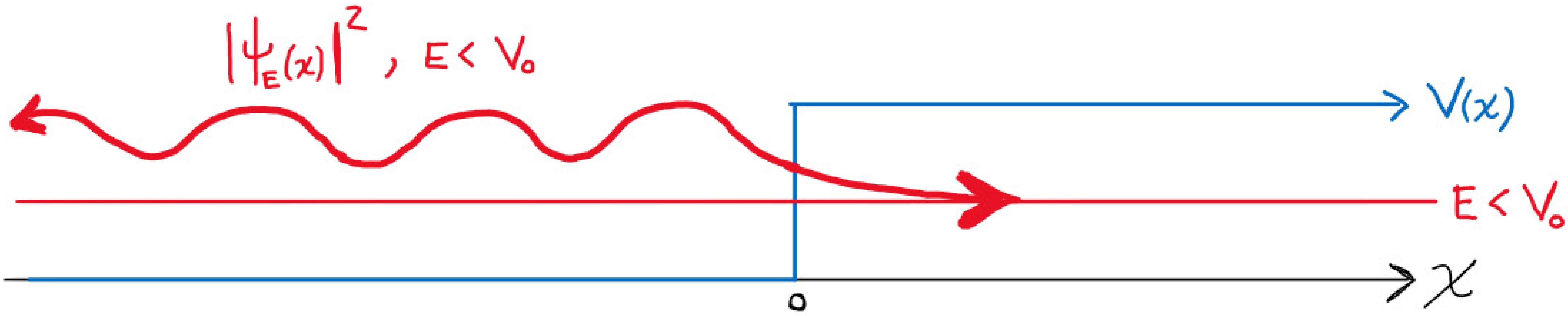


$x \geq 0$: $\quad \mathrm{Im}\left(\psi^* \frac{d}{dx}\psi\right) = 0 \implies J_> = 0.$

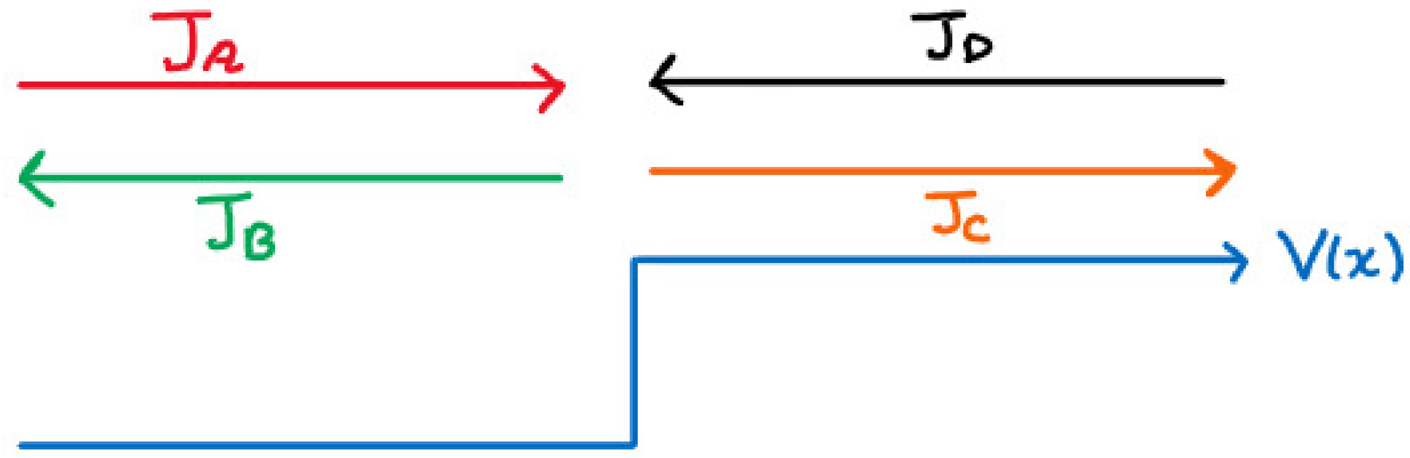
NO TRANSMISSION ! ONLY EXP. DECAY ("EVANESCENT") INTO BARRIER

DEFINE:

- REFLECTION COEFFICIENT : $R \equiv \frac{J_R}{J_I} = \left|\frac{B}{A}\right|^2 = 1$ HERE: PERFECT REFL. OF INCIDENT PROBABILITY FLUX FOR $E < V_0$.



b) $E \geq V_0$: Finite Transmission over Step Potential



$$\psi_<(x) = A e^{iK_1 x} + B e^{-iK_1 x} \; ; \quad K_1 = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} > 0$$

$$\psi_>(x) = C e^{iK_2 x} + D e^{-iK_2 x} \; ; \quad K_2 = \left[\left(\frac{2m}{\hbar^2}\right)(E - V_0)\right]^{1/2}$$

$$J_<(x) = \frac{\hbar K_1}{m}\left(|A|^2 - |B|^2\right) ; \quad J_>(x) = \frac{\hbar K_2}{m}\left(|C|^2 - |D|^2\right)$$

Continuity Conditions:
$$A + B = C + D$$
$$iK_1(A - B) = iK_2(C - D)$$
$\Rightarrow$ Matrix Form: $\begin{bmatrix} 1 & 1 \\ iK_1 & -iK_1 \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ iK_2 & -iK_2 \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix}$

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ iK_1 & -iK_1 \end{bmatrix}^{-1}\begin{bmatrix} 1 & 1 \\ iK_2 & -iK_2 \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix} = \frac{1}{-2iK_1}\begin{bmatrix} -iK_1 & -1 \\ -iK_1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ iK_2 & -iK_2 \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix} = \frac{1}{-2iK_1}\begin{bmatrix} -i(K_1+K_2) & i(K_2-K_1) \\ i(K_2-K_1) & -i(K_1+K_2) \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix}$$

Determines C, D in terms of A, B (or vice-versa)

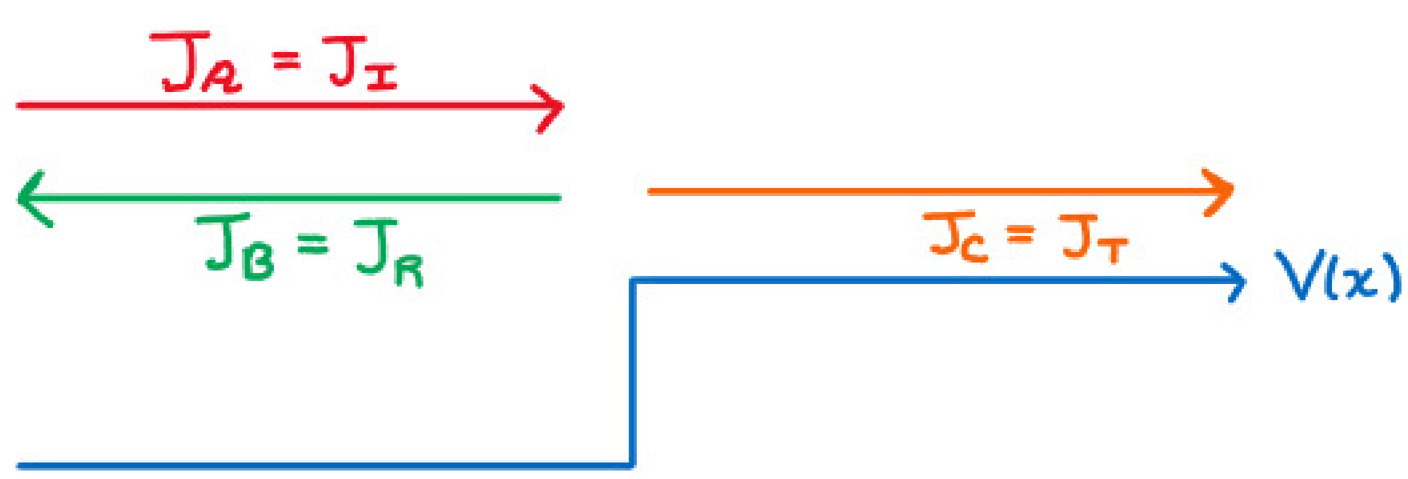
$\Rightarrow$ Still Two Complex Unknowns (Normalization, Overall Phase Fixes 1 Complex Constant)

2 Physical Solutions:

(1.) Left Incident:

Probability Flux propagates to Right from $x = -\infty$,

Reflects back, Transmits Forward



$\therefore$ Set $D = 0$.

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{-2iK_1}\begin{bmatrix} -i(K_1+K_2) & i(K_2-K_1) \\ i(K_2-K_1) & -i(K_1+K_2) \end{bmatrix}\begin{bmatrix} C \\ 0 \end{bmatrix} \qquad A = \frac{K_1+K_2}{2K_1}C \qquad B = \frac{K_1-K_2}{2K_1}C \quad \Rightarrow$$

$$\boxed{B = \left(\frac{K_1 - K_2}{K_1 + K_2}\right)A \qquad C = \left(\frac{2K_1}{K_1+K_2}\right)A}$$

Reflection Coefficient: $R = \frac{J_R}{J_I} = \left|\frac{B}{A}\right|^2 = \left(\frac{K_1 - K_2}{K_1 + K_2}\right)^2$

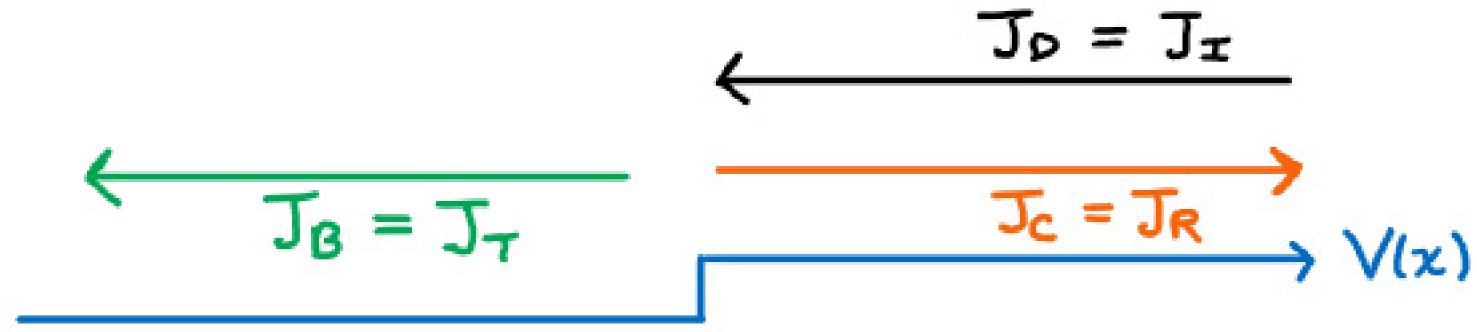
Transmission Coefficient: $T = \frac{J_T}{J_I} = \frac{\frac{\hbar K_2}{m}|C|^2}{\frac{\hbar K_1}{m}|A|^2} = \frac{K_2}{K_1}\left|\frac{C}{A}\right|^2 = \frac{4K_1K_2}{(K_1 + K_2)^2}$

Conservation of Probability Flux: $R + T = \left(\frac{K_1 - K_2}{K_1 + K_2}\right)^2 + \frac{4K_1K_2}{(K_1+K_2)^2} = 1$ ✓

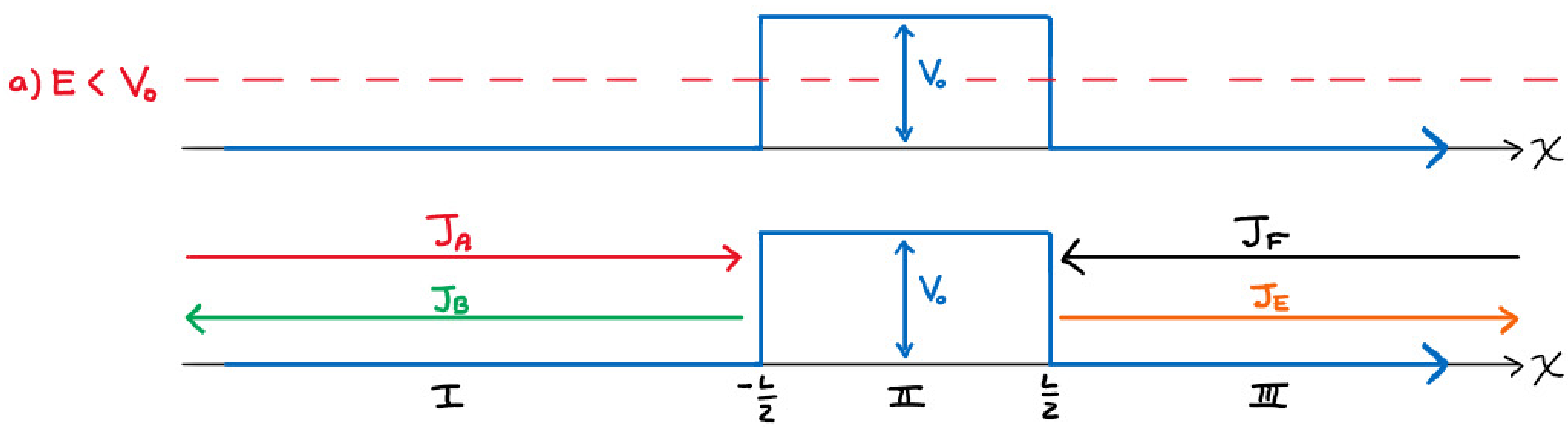
(2.) Right Incident

- $A = 0$

Need Both Left, Right-Inc. Eigenstates to Form Res. of Identity!



② Finite Step Barrier



$$\psi_{I}(x) = A e^{iK_1 x} + B e^{-iK_1 x} \quad ; \quad K_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2} \geq 0$$

$$\psi_{II}(x) = C e^{-K_2 x} + D e^{K_2 x} \quad ; \quad K_2 = \left(\frac{2m}{\hbar^2}\right)^{1/2} (V_0 - E)^{1/2} \geq 0$$

↑ Not excluded — finite interval

$$\psi_{III}(x) = E e^{iK_1 x} + F e^{-iK_1 x}$$

$$J_A = \frac{\hbar K_1}{m} |A|^2$$

$$J_B = \frac{\hbar K_1}{m} |B|^2$$

$$J_E = \frac{\hbar K_1}{m} |E|^2$$

$$J_F = \frac{\hbar K_1}{m} |F|^2$$

Let $e^{iK_1 \frac{L}{2}} \equiv \phi \; ; \; \phi^* = e^{-iK_1 \frac{L}{2}} = \phi^{-1} ; \quad e^{-K_2 \frac{L}{2}} \equiv \Theta$

Continuity:

I-II

$$\begin{bmatrix} \phi^* & \phi \\ iK_1\phi^* & -iK_1\phi \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \Theta^{-1} & \Theta \\ -K_2\Theta^{-1} & K_2\Theta \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}$$

II-III

$$\begin{bmatrix} \Theta & \Theta^{-1} \\ -K_2\Theta & K_2\Theta^{-1} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \phi & \phi^* \\ iK_1\phi & -iK_1\phi^* \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}$$

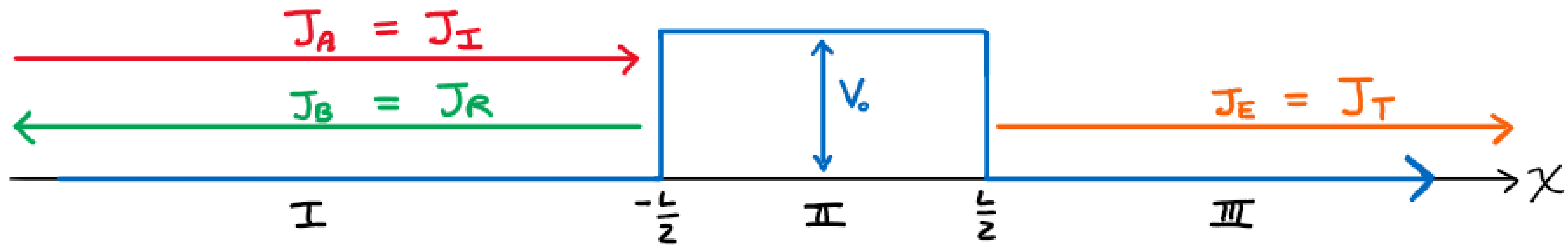
Define:

$$\hat{M}(\psi, q) \equiv \begin{bmatrix} \psi & \psi^{-1} \\ q\psi & -q\psi^{-1} \end{bmatrix}$$

$$\begin{bmatrix} A \\ B \end{bmatrix} = \hat{M}^{-1}(\phi^*, iK_1)\, \hat{M}(\Theta^{-1}, -K_2) \begin{bmatrix} C \\ D \end{bmatrix} \quad ; \quad \begin{bmatrix} C \\ D \end{bmatrix} = \hat{M}^{-1}(\Theta, -K_2)\, \hat{M}(\phi, iK_1) \begin{bmatrix} E \\ F \end{bmatrix}$$

$$\boxed{\begin{bmatrix} A \\ B \end{bmatrix} = \hat{M}^{-1}(\phi^*, iK_1)\, \hat{M}(\Theta^{-1}, -K_2)\, \hat{M}^{-1}(\Theta, -K_2)\, \hat{M}(\phi, iK_1) \begin{bmatrix} E \\ F \end{bmatrix} \equiv \hat{M}_T \begin{bmatrix} E \\ F \end{bmatrix}}$$

(1) Left Incident : $F = 0$



$$R = \frac{J_B}{J_A} = \left|\frac{B}{A}\right|^2 \; ; \quad T = 1 - R = \frac{J_E}{J_A} = \left|\frac{E}{A}\right|^2$$

$$\begin{bmatrix} A \\ B \end{bmatrix} = \hat{M}_T \begin{bmatrix} E \\ 0 \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} E \\ 0 \end{bmatrix}$$

$$\Rightarrow \quad A = M_{11} E \; ; \quad B = M_{21} E \quad \therefore \quad \frac{E}{A} = \frac{1}{M_{11}} = \frac{2 e^{-iK_1 L} K_1 K_2}{2 K_1 K_2 \cosh(K_2 L) - i (K_1^2 - K_2^2) \sinh(K_2 L)}$$

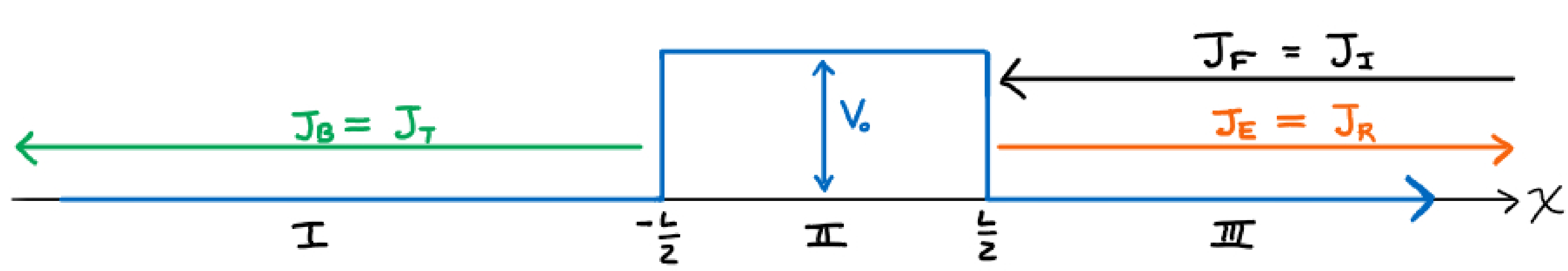
$$\frac{B}{A} = \frac{M_{21}}{M_{11}} = \frac{-i e^{-iK_1 L} (K_1^2 + K_2^2) \sinh(K_2 L)}{2 K_1 K_2 \cosh(K_2 L) - i (K_1^2 - K_2^2) \sinh(K_2 L)}$$

$$\therefore \quad T = \frac{(2K_1 K_2)^2}{(2K_1K_2)^2 \cosh^2(K_2 L) + (K_1^2 - K_2^2)^2 \sinh^2(K_2 L)}$$

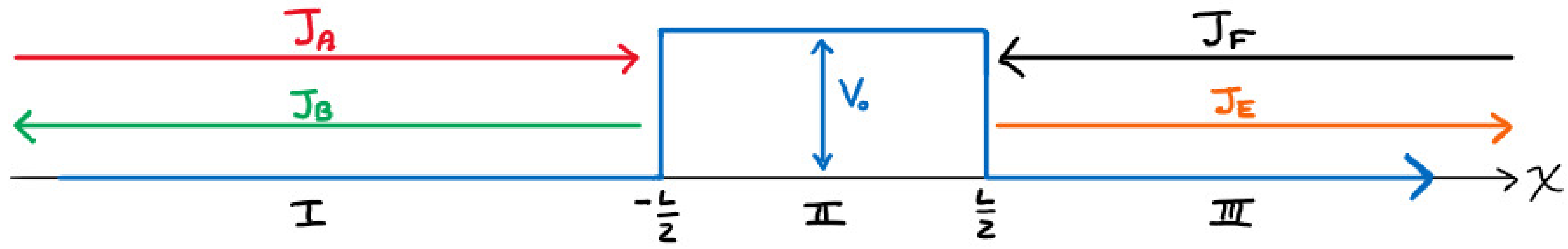
$$\therefore \quad R = \frac{(K_1^2 + K_2^2)^2 \sinh^2(K_2 L)}{(2K_1K_2)^2 \cosh^2(K_2 L) + (K_1^2 - K_2^2)^2 \sinh^2(K_2 L)}$$

$R + T = 1$ ✓

(2) Right-Incident : $A = 0$



$R = \frac{J_R}{J_I}$, $T = \frac{J_T}{J_I}$; Results are identical to the above due to parity symmetry, $[\hat{H}, \hat{\Pi}] = 0$ (HW 5, #2)



Summary: Eigenstates $(E < V_0)$

① Left-Incident

$$\psi^{(E<V_0)}_{K_1,L}(x) = \begin{cases} A\, e^{iK_1 x} + B\, e^{-iK_1 x}, & x < -\frac{L}{2} \\ C\, e^{-K_2 x} + D\, e^{K_2 x}, & |x| \le \frac{L}{2} \\ E\, e^{iK_1 x}, & x > \frac{L}{2} \end{cases}$$

$(K_1 \ge 0)$

- B, C, D, E completely determined by $\{A, K_1, K_2\}$
- A chosen to normalize

② Right-Incident

$$\psi^{(E<V_0)}_{K_1,R}(x) = \begin{cases} B\, e^{-iK_1 x}, & x < -\frac{L}{2} \\ C\, e^{-K_2 x} + D\, e^{K_2 x}, & |x| \le \frac{L}{2} \\ F\, e^{-iK_1 x} + E\, e^{iK_1 x}, & x > \frac{L}{2} \end{cases}$$

$(K_1 \ge 0)$

- B, C, D, E completely determined by $\{F, K_1, K_2\}$
- F chosen to normalize

- For $E \ge V_0$, must find associated L-, R-Incident Eigenstates $\psi^{(E \ge V_0)}_{K_1,L}$, $\psi^{(E \ge V_0)}_{K_1,R}$

Resolution of the Identity:

$K_1 = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} \Rightarrow K_1 = q \equiv \left(\frac{2mV_0}{\hbar^2}\right)^{\frac{1}{2}}$ marks transition between $(E < V_0)$, $(E \ge V_0)$ states.

$$\hat{\mathbb{I}} = \int_0^q dK_1 \left[\left|\psi^{(E<V_0)}_{K_1,L}\right\rangle\!\left\langle\psi^{(E<V_0)}_{K_1,L}\right| + \left|\psi^{(E<V_0)}_{K_1,R}\right\rangle\!\left\langle\psi^{(E<V_0)}_{K_1,R}\right| \right]$$

$$+ \int_q^\infty dK_1 \left[\left|\psi^{(E\ge V_0)}_{K_1,L}\right\rangle\!\left\langle\psi^{(E\ge V_0)}_{K_1,L}\right| + \left|\psi^{(E\ge V_0)}_{K_1,R}\right\rangle\!\left\langle\psi^{(E\ge V_0)}_{K_1,R}\right| \right]$$

Rather Complicated!