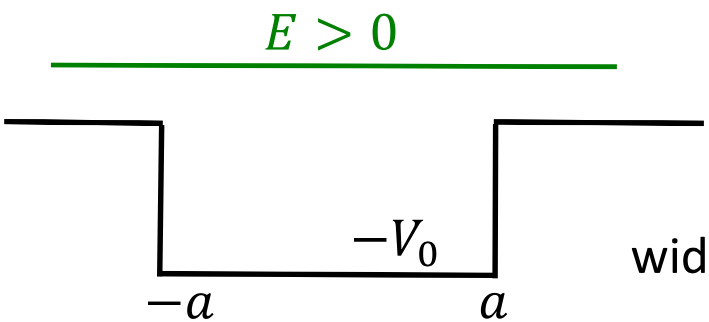
EE201/MSE207 Lecture 6

Finite square well: scattering states



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

width $2a$, depth V_0

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

Now E is given (any energy is possible)

Again 3 regions:

$x < -a$, $\psi(x) = A\,e^{ikx} + Be^{-ikx}$, $\quad k = \dfrac{\sqrt{2mE}}{\hbar}$ (definition of k as for free particle)

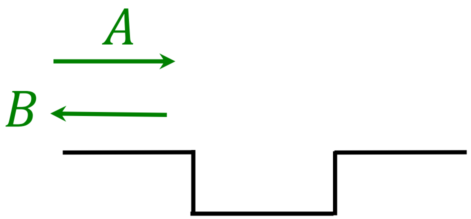
$|x| < a$, $\psi(x) = C\sin(lx) + D\cos(lx)$, $\quad l = \sqrt{2m(E+V_0)}/\hbar$ (as before)

$x > a$, $\psi(x) = F\,e^{ikx} + G\,e^{-ikx}$

4 boundary conditions, 6 variables (E is given, no normalization)
No hope to find unique solution. But there should not be a unique solution!
Let us focus on physical meaning (important to find a proper question).

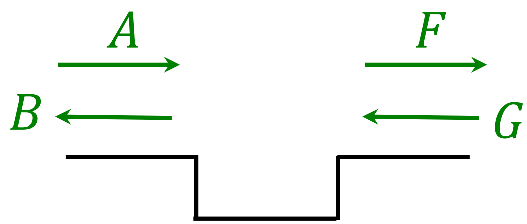
Add time dependence

$$x < -a, \qquad \Psi(x,t) = \underbrace{A\, e^{ik\left(x - \frac{\hbar k}{2m}t\right)}}_{\text{incident wave}} + \underbrace{B\, e^{-ik\left(x + \frac{\hbar k}{2m}t\right)}}_{\text{outgoing wave}}$$



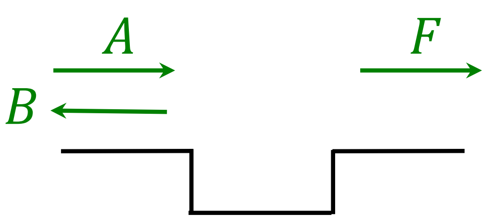
(as for free particle; different phase and group velocities, but the same direction)

Similarly for $x > a$



(if necessary, wave packets can be constructed later; in reality nobody usually does it because it is too complicated; instead, people work with unnormalized states)

Assume that the wave is incident from the left, then $G = 0$

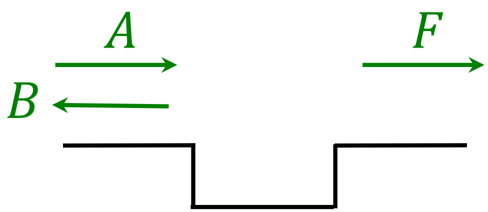


A is incident wave amplitude
B is reflected wave amplitude
F is transmitted wave amplitude

We have 5 variables (A, B, C, D, F) and 4 equations. Equations are linear.

Can express B, C, D, F as functions of A (incident amplitude).

Proper questions



A is incident wave amplitude
B is reflected wave amplitude
F is transmitted wave amplitude

(assume a wave incident from the left)

Goal: find ratios $r = \frac{B}{A}$ and $t = \frac{F}{A}$

(these ratios are called reflection and transmission amplitudes)

Reflection coefficient (probability of reflection) $R = |r|^2 = \frac{|B|^2}{|A|^2}$

Transmission coefficient (probability of transmission) $T = |t|^2 = \frac{|F|^2}{|A|^2}$

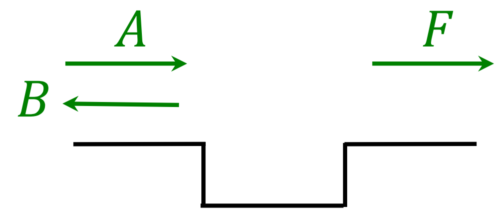
From physical meaning $T + R = 1$

Remark 1. Definition of T is sometimes different (discuss later, $\times\, v_r/v_l$)

Remark 2. Terminology: Reflection/transmission amplitudes (r, t)
and coefficients (R, T)

Remark 3. We defined R and T as ratios; they become probabilities for wave packets (possible to show). Quadratic because probability $\propto |\Psi|^2$.

Finding T and R



$$x < -a, \quad \psi(x) = A\, e^{ikx} + B\, e^{-ikx}$$

$$|x| < a, \quad \psi(x) = C \sin(lx) + D \cos(lx)$$

$$x > a, \quad \psi(x) = F\, e^{ikx}$$

Boundary conditions:

$$x = -a \quad \begin{cases} A\, e^{-ika} + B e^{ika} = -C \sin(la) + D \cos(la) \\ ik\left[A\, e^{-ika} - B e^{ika}\right] = l\, [C \cos(la) + D \sin(la)] \end{cases}$$

$$x = a \quad \begin{cases} C \sin(la) + D \cos(la) = F\, e^{ika} \\ l\, [C \cos(la) - D \sin(la) = ik\, F\, e^{ika} \end{cases}$$

Simple to exclude C and D (similar combinations), then 2 equations with A, B, F

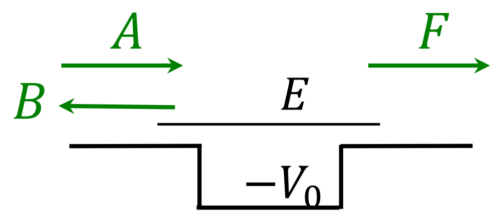
Finally

$$\begin{cases} F = \dfrac{e^{-2ika}}{\cos(2la) - i \dfrac{\sin(2la)}{2kl}(k^2 + l^2)} A \\ B = i \dfrac{\sin(2la)}{2kl}(l^2 - k^2)\, F \end{cases}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$l = \frac{\sqrt{2m(E + V_0)}}{\hbar}$$

Finding T and R



$$x < -a, \quad \psi(x) = A\, e^{ikx} + B\, e^{-ikx}$$

$$x > a, \quad \psi(x) = F\, e^{ikx}$$

Transmission probability

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}$$

Reflection probability

$$R = 1 - T$$

(too long from $|B|^2/|A|^2$)

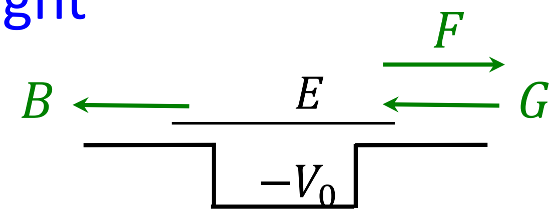
Remark. $T = 1$ if $\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi \iff E + V_0 = \frac{n^2\pi^2\hbar^2}{2m\,(2a)^2}$

This is exactly the "simple" energy quantization (in infinite well).

Explanation: destructive interference of reflected waves (similar to anti-reflective coating with quarter-wavelength films).

Now wave incident from the right

$$x < -a, \quad \psi(x) = B\, e^{-ikx}$$
$$x > a, \quad \psi(x) = F\, e^{ikx} + G\, e^{-ikx}$$



Similarly, we can find transmission and reflection coefficients

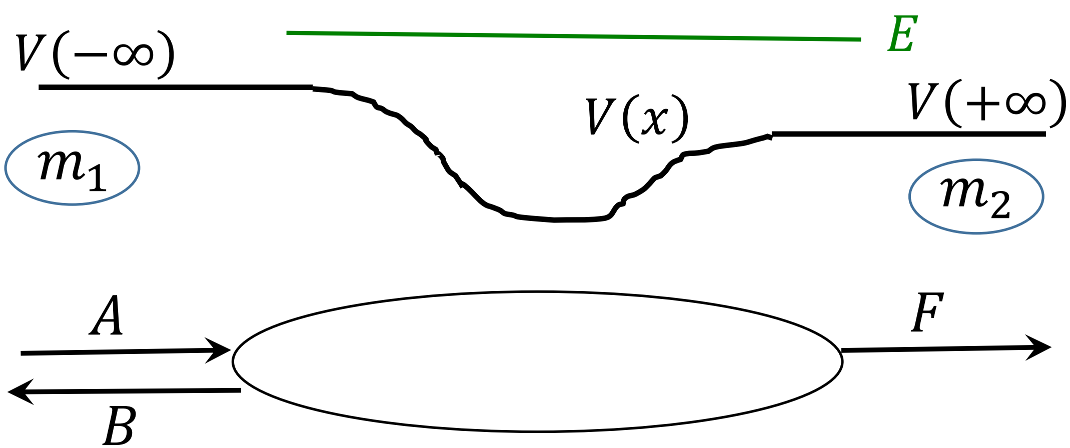
$$T_{\mathrm{r}} = |t_{\mathrm{r}}|^2 = \frac{|B|^2}{|G|^2} \qquad R_{\mathrm{r}} = |r_{\mathrm{r}}|^2 = \frac{|F|^2}{|G|^2} \qquad T_{\mathrm{r}} + R_{\mathrm{r}} = 1$$

In our case because of symmetry

$$T_{\mathrm{r}} = T_{\mathrm{l}} = T$$
$$R_{\mathrm{r}} = T_{\mathrm{l}} = R$$

However, this is always true (for any potential $V(x)$ and possibly different masses)

T and R in general case



$V(-\infty) \neq V(\infty)$
and/or $m_1 \neq m_2$

$$R = \frac{|B|^2}{|A|^2} = |r|^2$$

$$T + R = 1$$

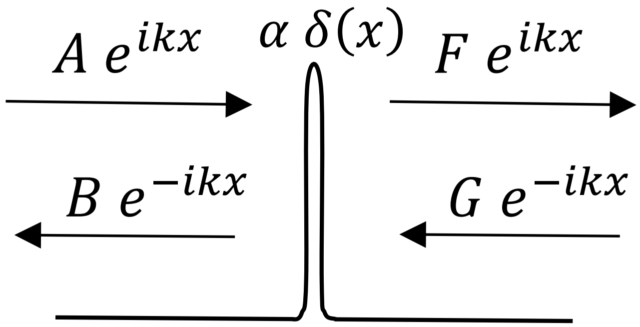
$$T = \frac{|F|^2}{|A|^2}\sqrt{\frac{E - V(+\infty)}{E - V(-\infty)}}\sqrt{\frac{m_1}{m_2}} = \frac{|F|^2}{|A|^2}\frac{k_2/m_2}{k_1/m_1} = \frac{|F|^2}{|A|^2}\frac{v_2}{v_1} = |t|^2\frac{v_2}{v_1}$$

Why? Probability current $J = \frac{i\hbar}{2m}\left(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx}\right)$ (remember that $m^{-1}\frac{d\psi}{dx}$ is continuous, not just $\frac{d\psi}{dx}$)

If $\psi(x) = A\, e^{ikx}$, then $J = |A|^2\frac{\hbar k}{m} = |A|^2 v$

The same velocity for reflection, but may be different for transmission

Transmission/reflection for δ-potential



$$V(x) = \alpha\,\delta(x)$$

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

$$E > 0$$

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

Integrate TISE near zero, $\int_{-\varepsilon}^{\varepsilon} \ldots$ $\Rightarrow$

$\varepsilon \to 0$

$$-\frac{\hbar^2}{2m}\left[\psi'(\varepsilon) - \psi'(-\varepsilon)\right] + \alpha\,\psi(0) = 0$$

$$\boxed{\frac{d\psi(+0)}{dx} - \frac{d\psi(-0)}{dx} = \frac{2m\alpha}{\hbar^2}\psi(0)}$$

With δ-potential, $d\psi/dx$ has a step (not continuous).

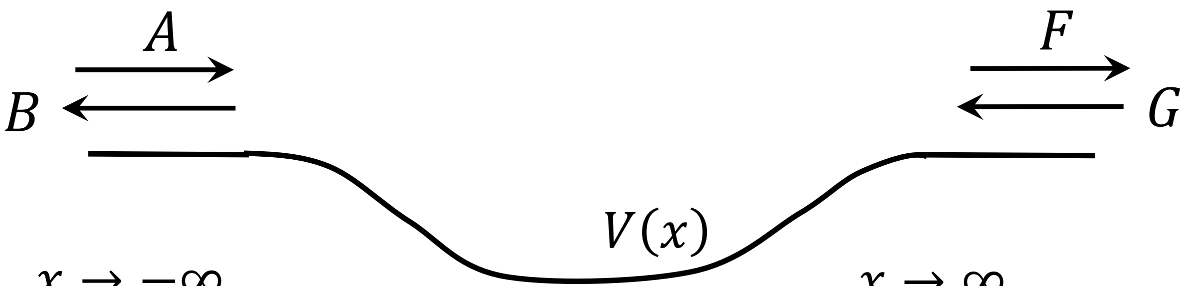
Boundary conditions
$$\begin{cases} A + B = F + G \\ ik(F-G) - ik(A-B) = \dfrac{2m\alpha}{\hbar^2}(A+B) \end{cases}$$

If $G = 0$ (incident from the left), then

$$\frac{B}{A} = \frac{-i\dfrac{m\alpha}{\hbar^2 k}}{1 + i\dfrac{m\alpha}{\hbar^2 k}}, \qquad \frac{F}{A} = \frac{1}{1 + i\dfrac{m\alpha}{\hbar^2 k}}$$

[not included into this course]

Scattering matrix (now waves incident from both sides)



For simplicity assume
$V(-\infty) = V(\infty)$,
$m_1 = m_2$

$x \to -\infty$

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

$x \to \infty$

$\psi(x) = Fe^{ikx} + Ge^{-ikx}$

Out of 4 wave amplitudes (A, B, F, G), 2 free parameters, and the other 2 can be calculated (linear relations)

Why 2 free parameters? 1) it was 2 in rectangular well
2) TISE is a second-order dif. eq. $\Rightarrow$ 2 boundary conditions

Suppose we found transmission/reflection amplitudes (t_l, r_l) for the wave incident from the left and also from the right (t_r, r_r).
It is convenient to write these 4 complex numbers as a 2×2 matrix.

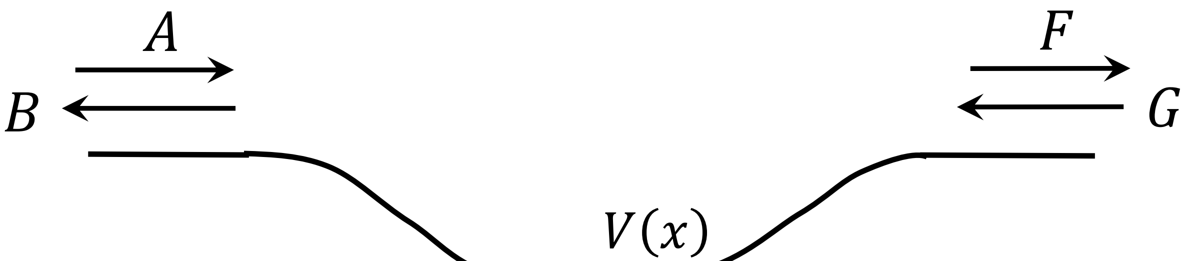
$$\hat{S} = \begin{pmatrix} r_l & t_r \\ t_l & r_r \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

(scattering matrix)

What is the meaning? $\begin{pmatrix} B \\ F \end{pmatrix} = \hat{S} \begin{pmatrix} A \\ G \end{pmatrix}$

(outgoing via incoming)

Scattering matrix (S-matrix)



For simplicity assume
$V(-\infty) = V(\infty)$,
$m_1 = m_2$

$x \to -\infty$

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

$x \to \infty$

$\psi(x) = Fe^{ikx} + Ge^{-ikx}$

$$\hat{S} = \begin{pmatrix} r_l & t_r \\ t_l & r_r \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

What is the meaning? $\begin{pmatrix} B \\ F \end{pmatrix} = \hat{S} \begin{pmatrix} A \\ G \end{pmatrix}$

(outgoing via incoming)

Suppose $G = 0$, then $\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} r_l A \\ t_l A \end{pmatrix}$ Suppose $A = 0$, then $\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} t_r G \\ r_r G \end{pmatrix}$

$T_l = |t_l|^2 = |S_{21}|^2, \quad R_l = |r_l|^2 = |S_{11}|^2$

$T_r = |t_r|^2 = |S_{12}|^2, \quad R_r = |r_r|^2 = |S_{22}|^2$

(remember that formulas for T in general case are different)

Let us prove symmetry: $\begin{cases} R_l = R_r \\ T_l = T_r \end{cases}$

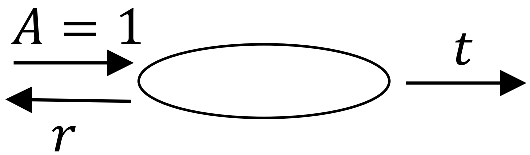
(for brevity will use notation: $t_l = t, r_l = r$)

Symmetry of the scattering matrix

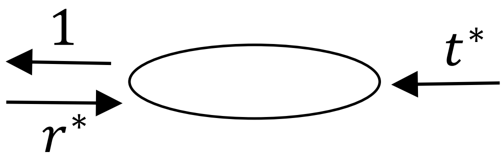
Our proof will use "graphical operations" with solutions of TISE

(conjugation = "time reversal")

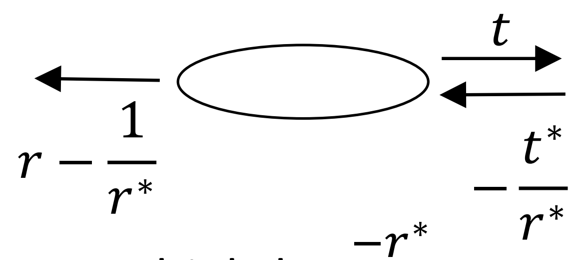
TISE



Conjugate solution of TISE

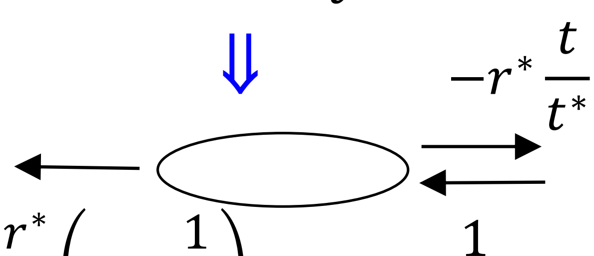


$+ \times \frac{-1}{r^*}$ $\Rightarrow$



Now multiply by $\frac{-r^*}{t^*}$

$\Downarrow$



$$\frac{-r^*}{t^*}\left(r - \frac{1}{r^*}\right) =$$

$$= \frac{1 - |r|^2}{t^*} = \frac{|t|^2}{t^*} = t$$

therefore

$$\begin{cases} t_r = t \\ r_r = -r^* \dfrac{t}{t^*} \end{cases}$$

$$\hat{S} = \begin{pmatrix} r & t \\ t & -r^* \dfrac{t}{t^*} \end{pmatrix}$$

$$\Rightarrow \begin{cases} T_r = T_l \\ R_r = R_l \end{cases}$$

Symmetry of the S-matrix in general case

$V(-\infty) \neq V(\infty),\ m_1 \neq m_2$

Without derivation, just a result

Still $\quad r_r = -r^* \dfrac{t}{t^*}$

(velocity v_1 at the left, v_2 at the right)

But $\quad t_r = \dfrac{1-|r|^2}{t^*} = \dfrac{|t|^2 \frac{v_2}{v_1}}{t^*} = t\,\dfrac{v_2}{v_1}$

$$\frac{v_2}{v_1} = \frac{k_2/m_2}{k_1/m_1}$$

$$\hat{S} = \begin{pmatrix} r & t\,\dfrac{v_2}{v_1} \\ t & -r^*\dfrac{t}{t^*} \end{pmatrix}$$

Then $\quad T_r = |t_r|^2 \dfrac{v_1}{v_2} = |t|^2 \dfrac{v_2}{v_1} = T_l$

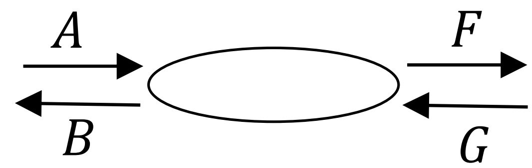
$R_r = R_l$

$\Rightarrow$ still $\begin{cases} T_r = T_l \\ R_r = R_l \end{cases}$

[also not included into this course]

Transfer matrix (*M*-matrix or *T*-matrix)

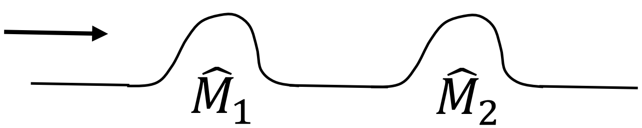
Sometimes instead of $\begin{pmatrix} B \\ F \end{pmatrix} = \hat{S} \begin{pmatrix} A \\ G \end{pmatrix}$



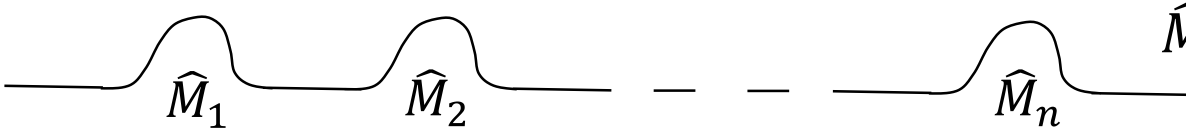
it is more convenient to use $\underbrace{\begin{pmatrix} F \\ G \end{pmatrix}}_{\text{right}} = \widehat{M} \underbrace{\begin{pmatrix} A \\ B \end{pmatrix}}_{\text{left}}$ (sometimes notation $\widehat{T}$ instead of $\widehat{M}$)

If we know $\hat{S}$, then it is easy to calculate $\widehat{M}$, and vice versa.

Why $\widehat{M}$ is convenient?



$$\widehat{M}_{\text{total}} = \widehat{M}_2\,\widehat{M}_1$$



$$\widehat{M}_{\text{total}} = \widehat{M}_n\,\widehat{M}_{n-1} \ldots \widehat{M}_1$$

For a multi-barrier structure, all $\widehat{M}_i$ are similar, therefore it is simple to calculate $\widehat{M}_{\text{total}}$. (Actually, each $\widehat{M}_i$ also contains a phase factor, depending on *x*-position.)

M-matrix: symmetries and relation to S-matrix

(simple case, $v_1 = v_2$)

Symmetries of M-matrix

1) $M_{22} = M_{11}^*$
2) $M_{12} = M_{21}^*$
3) $\det \widehat{M} = 1$

(can be derived from symmetries of S-matrix)

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix} \qquad \begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

Conversion

$$S_{11} = -\frac{M_{21}}{M_{22}} = -\frac{M_{12}^*}{M_{22}}$$

$$S_{22} = \frac{M_{12}}{M_{22}}$$

$$S_{12} = S_{21} = \frac{1}{M_{22}}$$

$$M_{11} = \frac{1}{S_{12}^*} = \frac{1}{S_{21}^*}$$

$$M_{22} = \frac{1}{S_{12}}$$

$$M_{12} = -\frac{S_{11}^*}{S_{12}^*} = \frac{S_{22}}{S_{12}}$$

$$M_{21} = -\frac{S_{11}}{S_{12}}$$