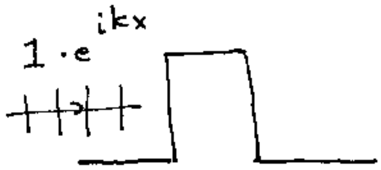
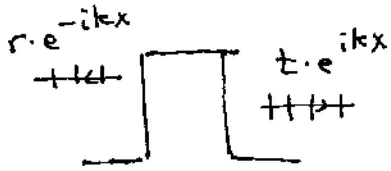
The $\mathcal{S}$-matrix (Heisenberg 1942)

In our examples of scattering we had a specified incident plane wave of unit strength and the most general possible final state (transmitted & reflected):





ψ_i $\qquad\qquad\qquad$ ψ_f

$$\psi_{tot} = \psi_i + \psi_f$$

All we really need to specify the situation are the coefficients of the incident and final waves, $1;\ r, t$.

We can write the entire effect of the potential $V(x)$ as seen from an observer at $x \to \pm\infty$ as a matrix that gives the final coeffs in terms of the initial ones:

$$\underset{\text{(incoming)}}{\textbf{init}}\ \text{wfn} = \underbrace{\overbrace{c_R^i}^{\text{right-moving}}}_{1} \cdot e^{ikx} + \underbrace{\overbrace{c_L^i}^{\text{left-moving}}}_{0} \cdot e^{-ikx} \qquad |i\rangle = \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix} = \underbrace{\begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{\text{our e.g.}}$$

which scatters into

$$\underset{\text{(outgoing)}}{\textbf{final}}\ \text{wfn} = \underbrace{\overbrace{c_R^f}^{\text{right-moving}}}_{t} e^{ikx} + \underbrace{\overbrace{c_L^f}^{\text{left-moving}}}_{r} e^{-ikx} \qquad |f\rangle = \begin{bmatrix} c_R^f \\ c_L^f \end{bmatrix} = \overbrace{\begin{bmatrix} t \\ r \end{bmatrix}}$$

So, the final amplitudes in terms of the initial amplitude(s) are

fin = matrix · init

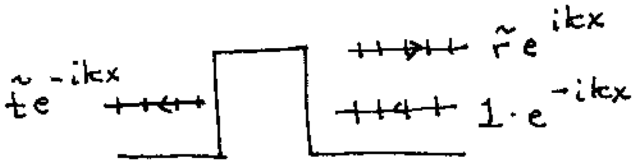
$$\begin{bmatrix} c_R^f \\ c_L^f \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{S}_{11} & \mathcal{S}_{12} \\ \mathcal{S}_{21} & \mathcal{S}_{22} \end{bmatrix}}_{\text{the } \mathcal{S}\text{-matrix}} \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix} \qquad \underbrace{\begin{bmatrix} t \\ r \end{bmatrix} = \begin{bmatrix} t & \cdot \\ r & \cdot \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{\text{what we know about our e.g. thus far}}$$

This contains the result of all possible scat. expts.
<u>The $\mathcal{S}$-matrix is everything measurable</u>!

$$\begin{bmatrix} c_R^f \\ c_L^f \end{bmatrix} = \underbrace{\begin{bmatrix} t & \cdot \\ r & \cdot \end{bmatrix}}_{\mathcal{S} = \begin{bmatrix} t & \tilde{r} \\ r & \tilde{t} \end{bmatrix}} \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix}$$

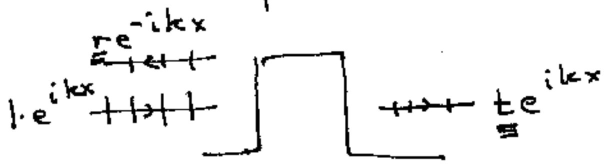
<u>What about the other entries in the $\mathcal{S}$-matrix?</u>

We need to concider scattering from the potential for an incident plane wave from the left;



$|f\rangle = \begin{bmatrix} \tilde{r} \\ \tilde{t} \end{bmatrix}$ $\quad$ $|i\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ $\qquad$ (1)

we <u>could</u> solve the Schrö. eqn. explicitly, but often one can use the previous solution of



(2)

to infer the new coefficients.

One way: <u>parity</u>. If $V(x) = V(-x)$ (you may have to shift your coordinates), $\psi(-x)$ is <u>also</u> a soln of the Schrö equn.

<u>proof</u>

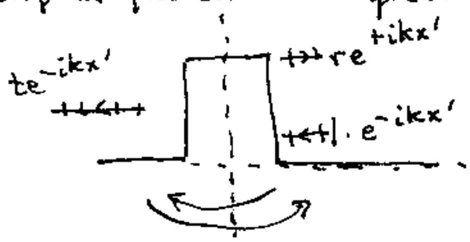
$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)$$

change vars to $x' = -x$, $\quad \frac{d^2}{dx^2} = (-)^2\frac{d^2}{dx'^2}$

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

if $=V(x')$, then $\psi(-x') \to \psi(-x)$ is also a soln.

parity on the original problem (2) gives



x'

(3)

which solves (1).

$\tilde{t} = t$, $\tilde{r} = r$, so $\mathcal{S}$ is

$$\begin{bmatrix} c_R^f \\ c_L^f \end{bmatrix} = \begin{bmatrix} t & \tilde{r} \\ r & \tilde{t} \end{bmatrix} \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix} = \underbrace{\begin{bmatrix} t & r \\ r & t \end{bmatrix}}_{\text{the full } \mathcal{S}\text{-matrix for this problem.}} \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix}$$

$$\underline{|f\rangle \equiv \mathcal{S}|i\rangle}$$

<u>Unitarity of the $\mathcal{S}$-matrix</u>

Conservation of probability says no particles lost in scat. $\underbrace{|c_R^f|^2 + |c_L^f|^2}_{\langle f|f\rangle} = \underbrace{|c_R^i|^2 + |c_L^i|^2}_{\langle i|i\rangle}$,

(just in case you aren't used to the notation,

$$|i\rangle = \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix} \qquad \langle i| = \begin{bmatrix} c_R^{i*} & c_L^{i*} \end{bmatrix}$$

$$\langle i|i\rangle = \begin{bmatrix} c_R^{i*} & c_L^{i*} \end{bmatrix} \begin{bmatrix} c_R^i \\ c_L^i \end{bmatrix} = |c_R^i|^2 + |c_L^i|^2 \quad)$$

$(=1)$.

Since $|f\rangle = \mathcal{S}|i\rangle$ this says

$$\langle f|f\rangle = \langle i|\mathcal{S}^\dagger \mathcal{S}|i\rangle = \langle i|i\rangle \qquad \forall\ |i\rangle$$

hence $\mathcal{S}^\dagger \mathcal{S} = I$, <u>the $\mathcal{S}$-matrix is unitary ($\mathcal{S}^\dagger = \mathcal{S}^{-1}$).</u>

What does unitarity imply?

Consider our e.g.

$$S = \begin{bmatrix} t & r \\ r & t \end{bmatrix} \qquad \underset{\underset{S^{T*}}{\shortparallel}}{S^{\dagger}} = \begin{bmatrix} t^* & r^* \\ r^* & t^* \end{bmatrix} = S^{-1}$$

n.b. S on-diagonal = unmodified state
off-diag. = scattered into diff. states.

$S = I$ is no scattering.

people often write $S = I + i\underbrace{T}$

"T-matrix", transition matrix,
to calculate the nontrivial part
of the scattering problem.

unitarity

$$S^{\dagger} S = I$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} t^* & r^* \\ r^* & t^* \end{bmatrix} \begin{bmatrix} t & r \\ r & t \end{bmatrix} = \begin{bmatrix} |r|^2 + |t|^2 & rt^* + r^* t \\ r^* t + r t^* & |r|^2 + |t|^2 \end{bmatrix}$$

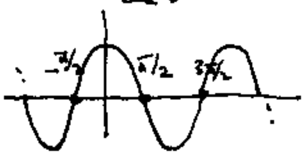
or $|r|^2 + |t|^2 = 1$ ✓ cons. of probability or flux – we already know this

$rt^* + r^* t = 0$ a new constraint!

If r & t are nonzero, since they are complex in general,

$$r = |r| e^{i\delta_r} \quad , \quad t = |t| e^{i\delta_t} \, ,$$

$$\underbrace{2|r||t|}_{\neq 0} \underbrace{\left(\frac{e^{i(\delta_r - \delta_t)} + e^{-i(\delta_r - \delta_t)}}{2} \right)}_{\cos(\delta_r - \delta_t)} = 0$$



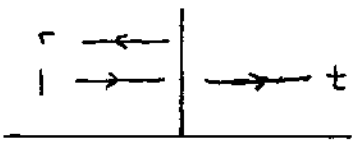
$\delta_r - \delta_t = (n + \frac{1}{2})\pi$, δ_r & δ_t are out of phase by 90°,

$\therefore$ r and t are <u>relatively imaginary</u>.

$$\frac{r}{t} = -\left(\frac{r}{t}\right)^* \quad \leftrightarrow \quad rt^* + r^* t = 0$$

(if nonzero)

A quick check of this. Recall our δ-potential prob,



$$t = \left(1 + \frac{i}{\kappa}\right)^{-1} \qquad \kappa \equiv \frac{\hbar^2 k}{m v_0}$$

$$r = -(1 - i\kappa)^{-1}$$

are t & r really 90° out of phase?
(ratio pure Im?)

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

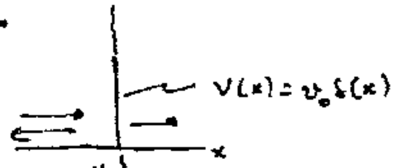
$$\frac{(r/t)^*}{(r/t)} = \frac{\left(1 - \frac{i}{\kappa}\right)}{(1 + i\kappa)} \cdot \frac{(1 - i\kappa)}{\left(1 + \frac{i}{\kappa}\right)} = \frac{(\kappa - i)}{(1 + i\kappa)} \cdot \frac{(1 - i\kappa)}{(\kappa + i)} = \frac{\cancel{(\kappa - i)}}{i\cancel{(\kappa - i)}} \cdot \frac{-i\cancel{(\kappa + i)}}{\cancel{(\kappa + i)}}$$

$$= -1 \quad \text{QED}$$

(reminder of the δ-potential scattering problem.)

Prob Set I

1.)



$\psi = e^{ikx} + r e^{-ikx} \;\big|\; t e^{ikx}$

a.) $-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$

$$\psi'' = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi$$

$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx \;\longrightarrow\; \psi'\Big|_{-\epsilon}^{\epsilon} = \frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon} v_0\,\delta(x)\psi(x)\,dx + O(\epsilon)$$

$$\lim_{\epsilon\to 0} \;\longrightarrow\; \psi'(\epsilon) - \psi'(-\epsilon) = \frac{2mv_0}{\hbar^2}\psi(0)$$

b.) b.c. ψ cont: $\quad 1 + r = t$

$$\psi' \text{ discont}: \quad \underset{\psi'(\epsilon)}{ikt} - \underset{\psi'(-\epsilon)}{ik(1-r)} = \frac{2mv_0}{\hbar^2}\underbrace{(1+r)}_{t}$$

c.) soln: $\quad 1 + r = t \qquad 1 - r = t\left(1 - \frac{2mv_0}{ik\hbar^2}\right) \equiv t\left(1 - \frac{2}{i\kappa}\right) \qquad \kappa \equiv \frac{\hbar^2 k}{m v_0}$

sum: $\quad 2 = t\left(2 - \frac{2}{i\kappa}\right), \quad t = \left(1 + \frac{i}{\kappa}\right)^{-1} = \frac{-i\kappa}{(1-i\kappa)}$

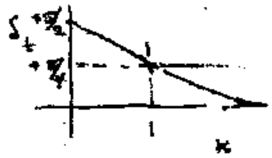
$$r = t - 1 = \frac{-1}{(1-i\kappa)}$$

d.) $P_t = |t|^2 = \frac{i\kappa}{(1+i\kappa)}\frac{(-i\kappa)}{(1-i\kappa)} = \frac{\kappa^2}{(1+\kappa^2)}$

$P_r = |r|^2 = \frac{1}{(1+\kappa^2)} \qquad P_r + P_t = |r^2| + |t^2| = \frac{\kappa^2}{(1+\kappa^2)} + \frac{1}{(1+\kappa^2)} = 1$ ✓

e.) $t = \left(1 + \frac{i}{\kappa}\right)^{-1} = |t|\, e^{i\delta_t}$

$$= \frac{\left(1 \mp \frac{i}{\kappa}\right)}{\left(1 + \frac{1}{\kappa^2}\right)} \qquad \therefore \tan\delta_t = -\frac{1}{\kappa}$$



This also explains our previous result for the finite square barrier with $E > V_0$, that when

$$r = \text{real} \implies t = \text{pure Im.}$$

It's another consequence of unitarity.

Block diagonals in S.

We can obviously calculate S in any basis we choose. The individual entries are

$$S_{ab} = \langle f | i \rangle$$

pure init and final basis states.

e.g. $S_{21} = \langle f_2 | i_1 \rangle = \langle 2 | \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} | 1 \rangle$ (or $\underline{\underline{S_{fi}}} = \langle f | i \rangle$ as a general matrix element)

$$= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} S_{11} \\ S_{21} \end{bmatrix} = S_{21} \checkmark$$

If there are conserved quantum numbers, scattering never takes you from an $|i\rangle$ state with one eigenvalue to a $|f\rangle$ with a different one. As an example, in potential scattering with a $V(r)$, ℓ is conserved, so if we write our initial wfn as

$$\psi_{init} = \sum_{\ell=0}^{\infty} c_\ell^i \underbrace{\psi_\ell(\vec{x})}_{(2\ell+1) i^\ell j_\ell(kr) P_\ell(\cos\theta) \text{ in our case}}$$

incoming coeffs $\quad |i\rangle = \begin{bmatrix} c_0^i \\ c_1^i \\ c_2^i \\ \vdots \\ (\infty) \end{bmatrix}$

Then the final coeff in each ℓ, c_ℓ^f must be proportional to c_ℓ^i only: the $\mathcal{S}$-matrix is diagonal! Note this does not mean it's unity. $\mathcal{S}^\dagger = \mathcal{S}^{-1}$ for $\mathcal{S}$ diagonal only implies that the entries are phases.

$$\mathcal{S} = \begin{bmatrix} e^{i\delta_0} & & & & \\ & e^{i\delta_1} & & & \\ & & e^{i\delta_2} & & \\ & & & \ddots & \\ & & & & e^{i\delta_\infty} \end{bmatrix}$$

[Where the $\{\delta_\ell\}$ are just the elastic scattering phase shifts.]

This is why we found that the coeff of $j_\ell P_\ell(\mu)$ in the scattering problem with $V(r)$ was simply multiplied by a phase, $e^{i\delta_\ell}$; ℓ is conserved and those are the only states with given ℓ.
[Actually we should be careful and separate ψ into incoming $\frac{e^{-ikr}}{r} P_\ell(\mu)$ and outgoing $\frac{e^{+ikr}}{r} P_\ell(\mu)$ waves to reach this conclusion.]

In a general problem in which several states share the same quantum numbers, e.g. $\{\psi_{A_1}, \psi_{A_2}\}$, $\{\psi_{B_1}, \psi_{B_2}, \psi_{B_3}\}$, the $\mathcal{S}$-matrix is block diagonal:

$$\mathcal{S} = \left[\begin{array}{c|c} \begin{array}{c}2\times 2\\ \text{A-block}\end{array} & 0 \\ \hline 0 & \begin{array}{c}3\times 3\\ \text{B-block}\end{array} \end{array}\right]$$

What do we find if we diagonalize $\mathcal{S}$? States that scatter into themselves.
[Energy eigenstates of the full H!]