SCATTERING AND S-MATRIX

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Part 1: Review of scattering theory	Part 2: S-matrix and related physics	Part 3: Some simple applications
S, T, and K matrices	1-,2-channel examples	Optical analogs
Wave packet scattering	Transmission resonances	Eikonal approximation
Scattering amplitude	Bound states	Diffractive scattering
Partial wave expansion	S wave properties	Adding resonances
Phase shifts	Resonances	Dalitz plot applications
R-matrix	Absorption	Historical notes
Unitarity circle	Inelastic cross section	Example from electronics

For simplicity some of the formalism will be nonrelativistic

"In" state $|i\rangle_{\rm in}$: Free particle in remote past

"Out" state ${}_{\rm out}\langle j|$: Free particle in remote future

S-matrix takes "in" states to "out" (with wave packets: Goldberger and Watson, *Scattering Theory*, 1964.)

UNITARITY; T AND K MATRICES

$S_{ji} \equiv_{\rm out} \langle j|i\rangle_{\rm in}$ is unitary: completeness and orthonormality of "in" and "out" states

$$S^\dagger S = S S^\dagger = \mathbb{1}$$

Just an expression of probability conservation

S has a piece corresponding to no scattering

Can write $S = \mathbb{1} + 2iT$

Notation of S. Spanier, BaBar Analysis Document #303, based on S. U. Chung *et al.* Ann. d. Phys. **4**, 404 (1995).

Unitarity of S-matrix $\Rightarrow T - T^\dagger = 2iT^\dagger T = 2iTT^\dagger$.

$(T^\dagger)^{-1} - T^{-1} = 2i\mathbb{1}$ or $(T^{-1} + i\mathbb{1})^\dagger = (T^{-1} + i\mathbb{1})$.

Thus $K \equiv [T^{-1} + i\mathbb{1}]^{-1}$ is hermitian; $T = K(\mathbb{1} - iK)^{-1}$

WAVE PACKETS

Normalized plane wave states: $\chi_{\vec{q}} = e^{i\vec{q}\cdot\vec{r}}/(2\pi)^{3/2}$

$$(\chi_{\vec{q}'}, \chi_{\vec{q}}) = (2\pi)^{-3} \int d^3\vec{r}\; e^{i(\vec{q}-\vec{q}')\cdot\vec{r}} = \delta^3(\vec{q}-\vec{q}')\ .$$

Expansion of wave packet: $\psi_{\vec{p}}(\vec{r}, t=0) = \int d^3q\, \chi_{\vec{q}}\, \phi(\vec{q}-\vec{p})$

where ϕ is a weight function peaked around 0

Fourier transform of ϕ: $G(\vec{r}) = \int d^3k\; e^{i\vec{k}\cdot\vec{r}} \phi(\vec{k})$

$$\psi_{\vec{p}}(\vec{r}, t=0) = \int d^3q\; \chi_{\vec{q}-\vec{p}+\vec{p}}\; \phi(\vec{q}-\vec{p}) = \chi_{\vec{p}}\, G(\vec{r})\ .$$

Norm: $(\psi, \psi) = \int d^3q\, |\phi(\vec{q}-\vec{p})|^2 = \frac{1}{(2\pi)^3} \int d^3r |G(\vec{r})|^2 = 1\,.$

$$\psi_{\vec{p}}(\vec{r}, t) = e^{-iHt} \psi_{\vec{p}}(\vec{r}, 0) = \int d^3q\; \phi(\vec{q}-\vec{p}) \chi_{\vec{q}} e^{-iE_q t}\ ,$$

where $E_q = q^2/2m$ (NR) or $(q^2+m^2)^{1/2}$ (Relativistic) .

WAVE PACKET SCATTERING

E. Merzbacher, *Quantum Mechanics* (3rd Ed. Ch. 13) has a good discussion which will be abbreviated here

Free Hamiltonian: $H_0 = p^2/(2m)$; full: $H = H_0 + V$

Packet: $\psi_{\vec{k}_0}(\vec{r}, 0) = \frac{1}{(2\pi)^{3/2}} \int d^3k \; \phi(\vec{k} - \vec{k}_0) e^{i\vec{k}\cdot(\vec{r} - \vec{r}_0)}$, $\phi(\vec{k})$ centered about 0, width Δk, center of packet $\vec{r}_0$

At $t = 0$ packet is headed to target, momentum $\vec{k}_0$, distance $\vec{r}_0$ from it; want its shape for large t

Expand $\psi_{\vec{k}_0}(\vec{r}, 0)$ in eigenfunctions of H:

$$\psi_{\vec{k}_0}(\vec{r}, 0) = \sum_n c_n \psi_n(\vec{r}) \quad , \quad \psi_{\vec{k}_0}(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r}) e^{-iE_n t} \, .$$

Need to find the eigenfunctions $\psi_n(\vec{r})$

GREEN'S FUNCTION

$\left(\frac{\vec{p}^2}{2m} + V\right)\psi = E\psi$, or with $k^2 \equiv 2mE$, $U \equiv 2mV$,

Schrödinger equation is $(\nabla^2 + k^2)\psi = U\psi$

Define a *Green's function* $G(\vec{r}, \vec{r'})$ satisfying

$$(\nabla^2 + k^2)G(\vec{r}, \vec{r'}) = -4\pi\delta(\vec{r} - \vec{r'})$$

$\psi(\vec{r}) = -\frac{1}{4\pi}\int d^3r'\ G(\vec{r}, \vec{r'})U(\vec{r'})\psi(\vec{r'})$: particular sol'n.

Add solution $e^{i\vec{k}\cdot\vec{r}}/(2\pi)^{3/2}$ of homogeneous equation:

$\psi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} - \frac{1}{4\pi}\int d^3r'\ G(\vec{r}, \vec{r'})U(\vec{r'})\psi_{\vec{k}}(\vec{r'})$

Differential eqn. + boundary condx. $\Leftrightarrow$ integral equation

SPHERICAL WAVES

Two Green's functions: $G_{\pm}(\vec{r},\vec{r'}) = \frac{e^{\pm ik|\vec{r}-\vec{r'}|}}{|\vec{r}-\vec{r'}|}$

with $(+,-) \Leftrightarrow$ (outgoing,incoming) spherical waves

Can take $\vec{r'} = 0$; $G_{\pm}$ are solutions for $\vec{r} \neq 0$

For $\vec{r} = 0$, integrate test function $f(\vec{r})$ times $(\nabla^2 + k^2)G$ over small region surrounding the origin; use Gauss' Law

Green's functions $G_{\pm}$ define two sets of solutions:

$$\psi^{(\pm)}_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} - \frac{1}{4\pi}\int d^3r' \, \frac{e^{\pm ik|\vec{r}-\vec{r'}|}}{|\vec{r}-\vec{r'}|} U(\vec{r'})\psi^{(\pm)}_{\vec{k}}(\vec{r'})$$

where r' is limited if U is of short range

Expand $k|\vec{r}-\vec{r'}| = k\sqrt{r^2 - 2\vec{r}\cdot\vec{r'} + r'^2} \simeq kr\left(1 - \frac{\vec{r}\cdot\vec{r'}}{r^2} + \ldots\right)$

$$1/|\vec{r} - \vec{r'}| \simeq 1/r$$

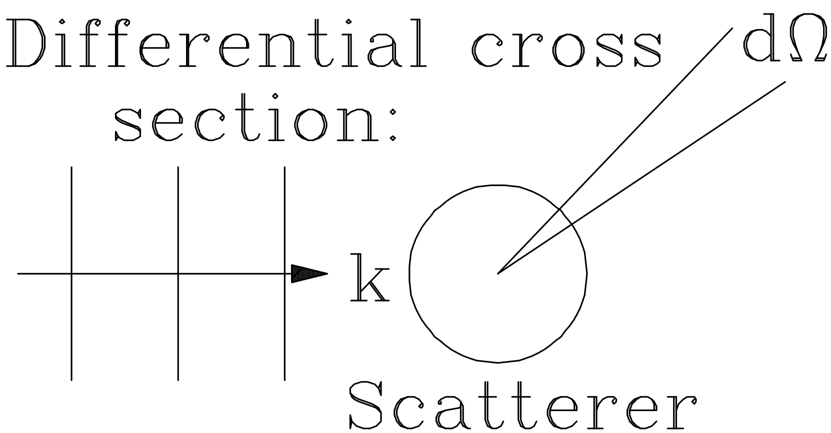
SCATTERING AMPLITUDE

$$\psi_{\vec{k}}^{(\pm)}(\vec{r}) \sim \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} - \frac{1}{4\pi r} e^{\pm ikr} \int d^3r'\, U(\vec{r'}) \psi_{\vec{k}}^{(\pm)}(\vec{r'}) e^{\mp i\vec{k'}\cdot\vec{r'}}$$

$$\vec{k'} \equiv k\hat{r}$$

Define $f_{\vec{k}}^{(\pm)}(\hat{r}) \equiv -\left[\frac{(2\pi)^{3/2}}{4\pi}\right] \int d^3r'\, U(\vec{r'}) \psi_{\vec{k}}^{(\pm)}(\vec{r'}) e^{\mp i\vec{k'}\cdot\vec{r'}}$

Then $\psi_{\vec{k}}^{(\pm)}(\vec{r}) \sim (2\pi)^{-3/2} \left[e^{i\vec{k}\cdot\vec{r}} + \frac{e^{\pm ikr}}{r} f_{\vec{k}}^{(\pm)}(\hat{r})\right] \quad (r \to \infty)$



Initial flux per unit area $I_0 \sim k$

Final fluence I
in cone of solid angle $d\Omega$:
$I \sim k(r^2 d\Omega)|f_{\vec{k}}^{(\pm)}(\hat{r})/r|^2$

$d\sigma/d\Omega = I/I_0 = |f_{\vec{k}}^{(\pm)}(\hat{r})|^2 \equiv$ differential cross section

PHASE SHIFTS δ_ℓ

Large-r Schr. eq. solution: $\psi \sim e^{ikr\cos\theta} + f_k(\theta)\frac{e^{ikr}}{r}$ (1)

Connect with central-force solutions $\frac{u_{\ell,k}(r)}{r}Y_\ell^m(\theta,\phi)$ where

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + 2mV(r) - k^2\right] u_{\ell,k}(r) = 0 \quad (k^2 \equiv 2mE)$$

Free $u_{\ell,k}(r)/r \equiv R_{\ell,k}(r)$ solutions $j_\ell(kr)$, $n_\ell(kr)$

Outside range of V: $R_{\ell,k}(r) = A_\ell\, j_\ell(kr) + B_\ell\, n_\ell(kr)$

As $kr \to \infty$ $R_{\ell,k}(r) \to A_\ell \frac{\sin(kr-\ell\pi/2)}{kr} - B_\ell \frac{\cos(kr-\ell\pi/2)}{kr}$

For $\tan\delta_\ell \equiv -B_\ell/A_\ell$, $R_{\ell,k}(r) \sim \frac{\sin(kr-\ell\pi/2+\delta_\ell)}{kr}$ as $kr \to \infty$

Then $\psi \to \sum C_\ell(k) P_\ell(\cos\theta)[\sin(kr - \ell\pi/2 + \delta_\ell)]/r$ (2)

Bauer: $e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell\, (2\ell+1) j_\ell(kr) P_\ell(\cos\theta)$ (3)

PARTIAL WAVE EXPANSION

Compare incoming spherical wave coefficients in (2,3):

$\psi \simeq \sum_{\ell=0}^{\infty}(2\ell+1)i^{\ell}e^{i\delta_\ell}[\sin(kr-\ell\pi/2+\delta_\ell)]P_\ell(\cos\theta)/kr$

Compare coeff. of outgoing spherical wave in this and (1):

$$f_k(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)[(e^{2i\delta_\ell(k)}-1)/(2ik)]P_\ell(\cos\theta)$$
$$= k^{-1}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell(k)}\sin\delta_\ell(k)P_\ell(\cos\theta)$$

Total cross section:

$$\sigma = \int d\Omega\,\frac{d\sigma}{d\Omega} = \int d\Omega\,|f_k(\theta)|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(k)$$

using $\int d\Omega\; P_\ell(\cos\theta)P_{\ell'}(\cos\theta) = 4\pi\delta_{\ell\ell'}/(2\ell+1)$

Optical theorem: $\sigma = (4\pi/k)\mathrm{Im}\; f_k(0)$

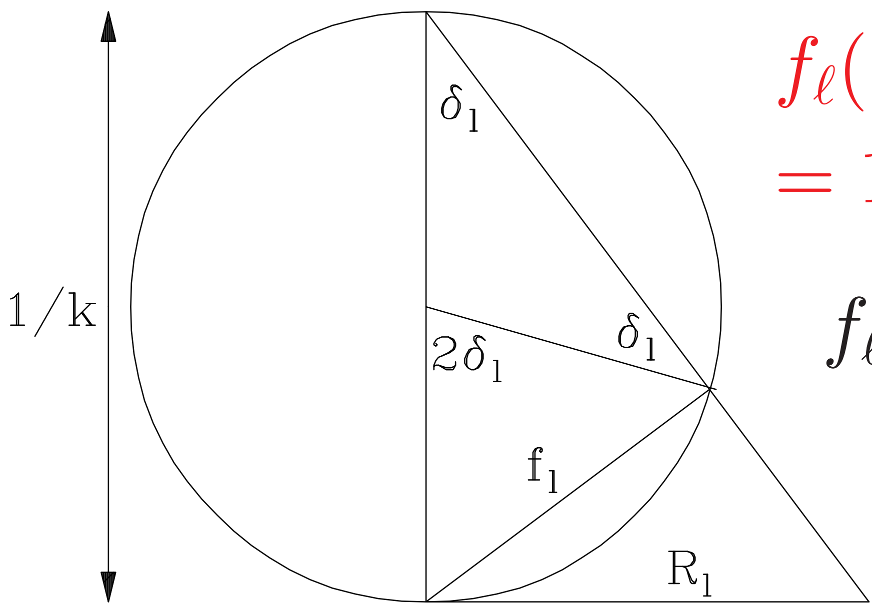
Convenient to define $f_\ell(k) \equiv [e^{2i\delta_\ell(k)}-1]/(2ik)$

Then optical theorem takes the form Im $f_\ell(k) = k|f_\ell(k)|^2$

THE R-MATRIX

Want a *real* function reducing to $f_\ell(k)$ for small f

Stereographic projection: $R_\ell(k) \equiv (1/k)\tan\delta_\ell(k)$



$f_\ell(k) = k^{-1} e^{i\delta_\ell(k)} \sin\delta_\ell(k)$

$= 1/k$ (maximum) for $\delta_\ell(k) = \pi$

$$f_\ell(k) = \frac{[1+ikR_\ell(k)]R_\ell(k)}{1+k^2R_\ell^2(k)}$$

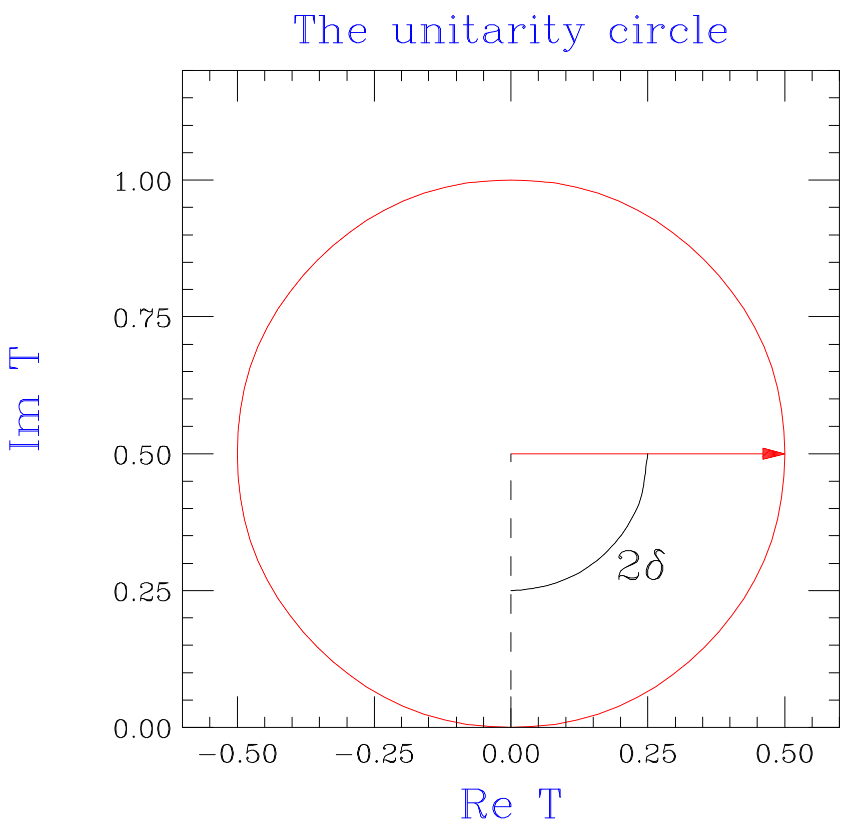
$$S_\ell(k) \equiv e^{2i\delta_\ell(k)} = \frac{1+ikR_\ell(k)}{1-ikR_\ell(k)}$$

Many channels: real R is useful because it has eigenvalues

S-matrix is useful because it is unitary: $S^\dagger S = 1$

$$S = \mathbb{1} + 2iT = (\mathbb{1} + iK)/(\mathbb{1} - iK)$$

UNITARITY CIRCLE



For single channel, phase shift defined by $S = e^{2i\delta}$.

Then $T = (S - \mathbb{1})/(2i) = e^{i\delta} \sin\delta$; $K = \tan\delta = kR$.

The T amplitude must lie on boundary of the circle

For inelastic processes

$T = (\eta e^{2i\delta} - \mathbb{1})/(2i)\ , \quad \eta < 1.$

Consider scattering in one dimension with no reflections

Class of potentials giving rise to full transmission of a plane wave $\psi(x) \sim e^{ikx}$ incident from the left, so that as $x \to \infty$, $\psi(x) \to S(k)e^{ikx}$ with $|S(k)| = 1$. Take $2m = 1$.

1,2–CHANNEL EXAMPLES

These potls. have bound states at energies $E_j = -\alpha_j^2$ $(1 \leq j \leq N$ and one can write $S(k) = \Pi_{j=1}^N[(ik - \alpha_j)/(ik + \alpha_j)] = e^{2i\delta}$, where $\delta = \sum_{j=1}^N \delta_j$ and $\tan\delta_j = \alpha_j/k$.

Simplest one-level potential: $V(x) = -2\alpha^2/\cosh^2\alpha(x - x_0)$

One-level K-matrix is just $K = \alpha/k$. If we define $K_j = \alpha_j/k$ then $K \to \sum_{j=1}^N K_j$ as $k \to \infty$, but not in general.

Now let the potential permit reflections, so that

$$\psi(x) \to Ae^{ikx} + Be^{-ikx} \quad (x \to -\infty)$$
$$\psi(x) \to Fe^{ikx} + Ge^{-ikx} \quad (x \to \infty)$$

With channel 1 $\sim e^{ikx}$, channel 2 $\sim e^{-ikx}$, can write

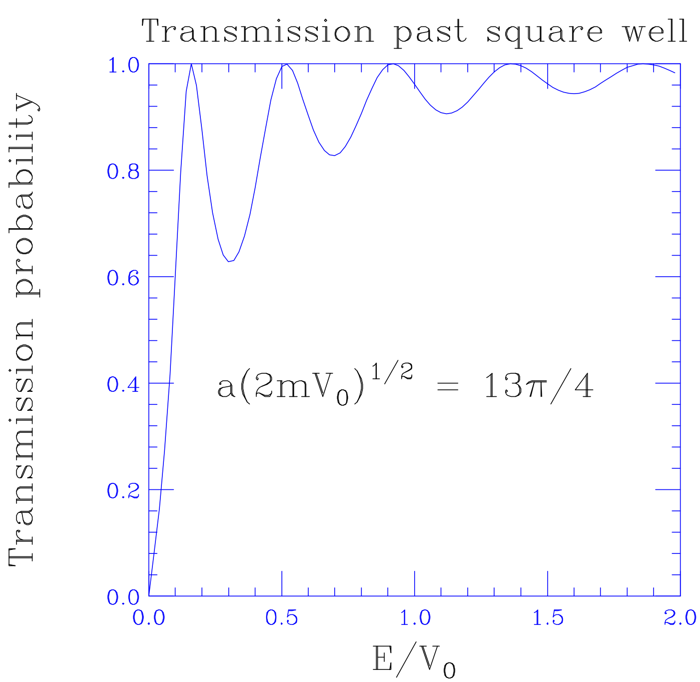
$$F = S_{11}A + S_{12}G \; ; \quad B = S_{21}A + S_{22}G$$

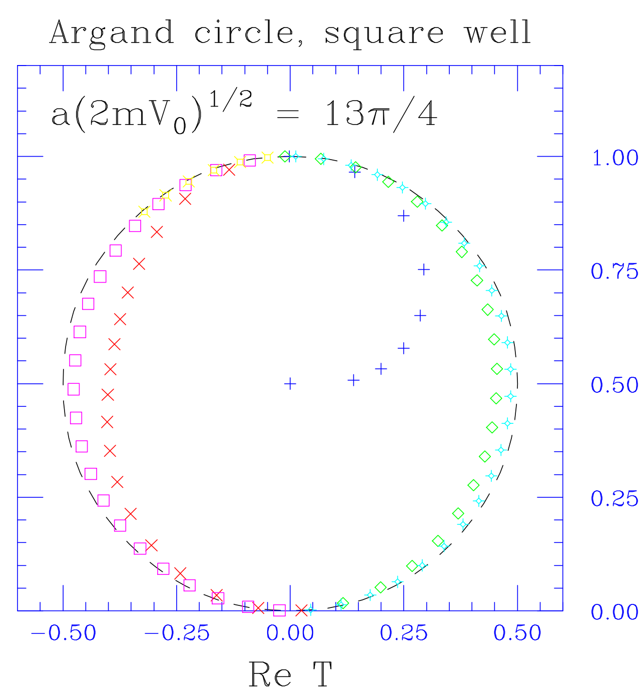
TRANSMISSION RESONANCES

The incoming and outgoing fluxes must be equal: $|F|^2 + |B|^2 = |A|^2 + |G|^2$. This implies $S^\dagger S = S S^\dagger = 1$.

Square well, $V(x) = -V_0$ for $|x| \leq a$, $V(x) = 0$ for $|x| > a$ shows transmission resonances: $|S_{11}| = |S_{22}| = 1$ and $S_{12} = S_{21} = 0$ when $2k'a = n\pi$ ($k' = \sqrt{2m(E+V_0)}$).

Merzbacher, *Quantum Mechanics* (3rd ed.), p. 109:



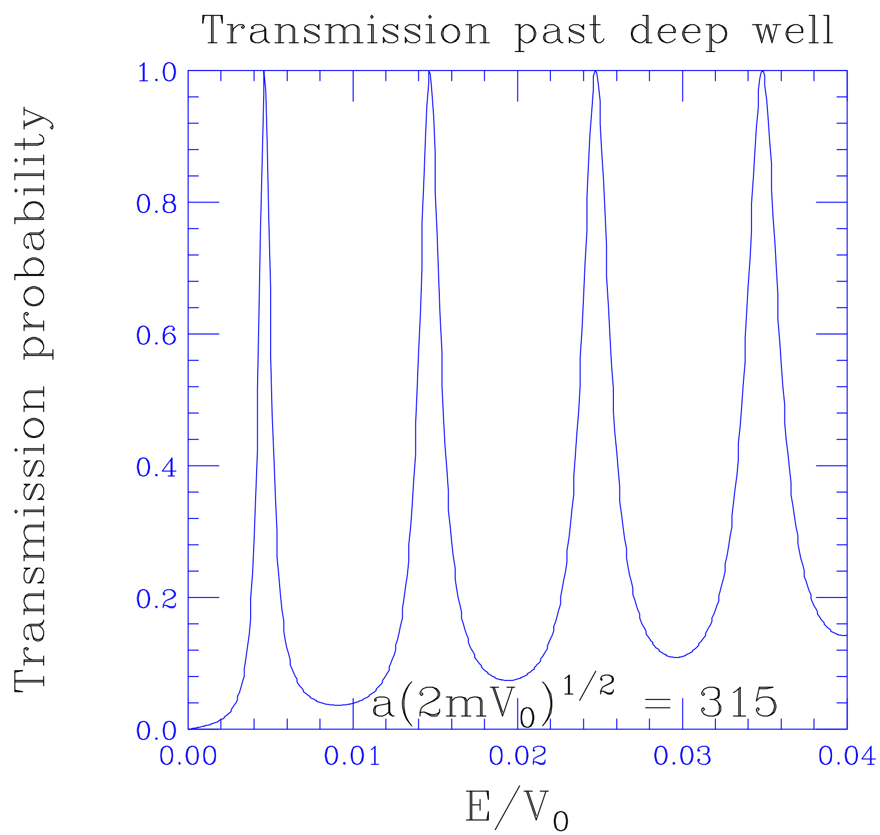


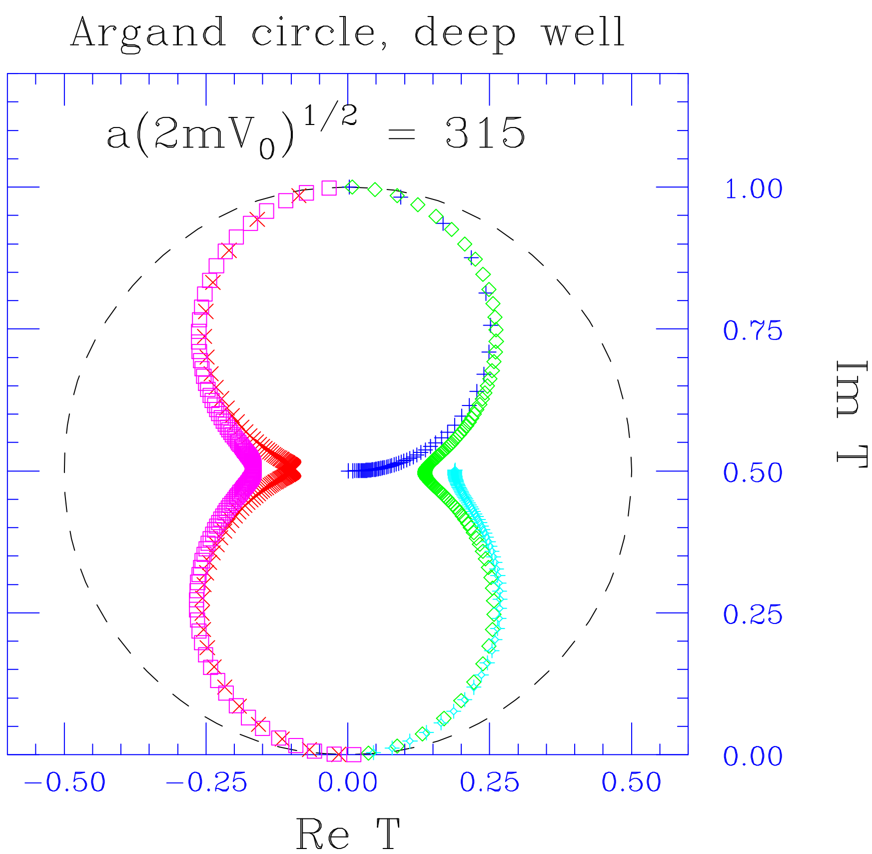
$S_{11} = S_{22} = \eta e^{2i\delta}$,
$iS_{12} = iS_{21} = \sqrt{1-\eta^2} e^{2i\delta}$.

Ticks: equal $\Delta E/V_0$ intervals

DEEP WELL EXAMPLE

Another example from Merzbacher, 3rd ed., p. 109.





Well much deeper; resonances more closely spaced in E.

S-MATRIX POLES AND BOUND STATES

Write reflectionless $S(k) = \Pi_{j=1}^{N}\left[\frac{i-\alpha_j/k}{i+\alpha_j/k}\right] = \frac{F(k)}{F(-k)} = e^{2i\delta}$

$F(k) = \Pi_{j=1}^{N}(i - \alpha_j/k)$ is an example of a *Jost function*

Zeroes of Jost function at $k = -i\alpha_j$ correspond to S-matrix poles at $k = i\alpha_j$ (bound states): wave function $e^{ikx} \rightarrow e^{-\alpha_j x}$ as $x \rightarrow \infty$ and $e^{-ikx} \rightarrow e^{\alpha_j x}$ as $x \rightarrow -\infty$

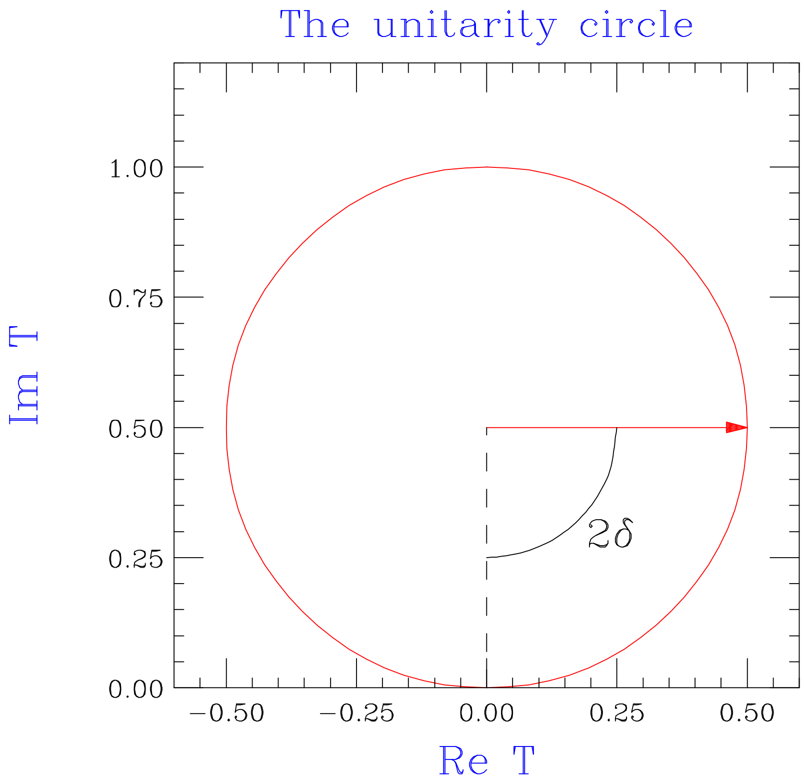
Phase of the Jost function is just the phase shift

Generalizes to all ℓ: $S_\ell(k) = F_\ell(k)/F_\ell(-k) = e^{2i\delta_\ell}$

R. Newton, J. Math. Phys. **1**, 319 (1960); P. Roman, *Advanced Quantum Theory*, Addison-Wesley, 1964

Useful in proving Levinson's Theorem: $\delta_\ell(k=0) - \delta(k=\infty) = n_\ell \pi$, where n_ℓ is the number of bound states with angular momentum ℓ

RAMSAUER-TOWNSEND EFFECT



S-wave scattering amplitude $f_0(k) = (e^{2i\delta} - 1)/(2ik)$ vanishes at $\delta = \pi$; $\sigma_{\rm el} = 0$ there

This is seen in scattering of electrons on rare gas atoms where $\sigma \simeq 0$ around 1 eV

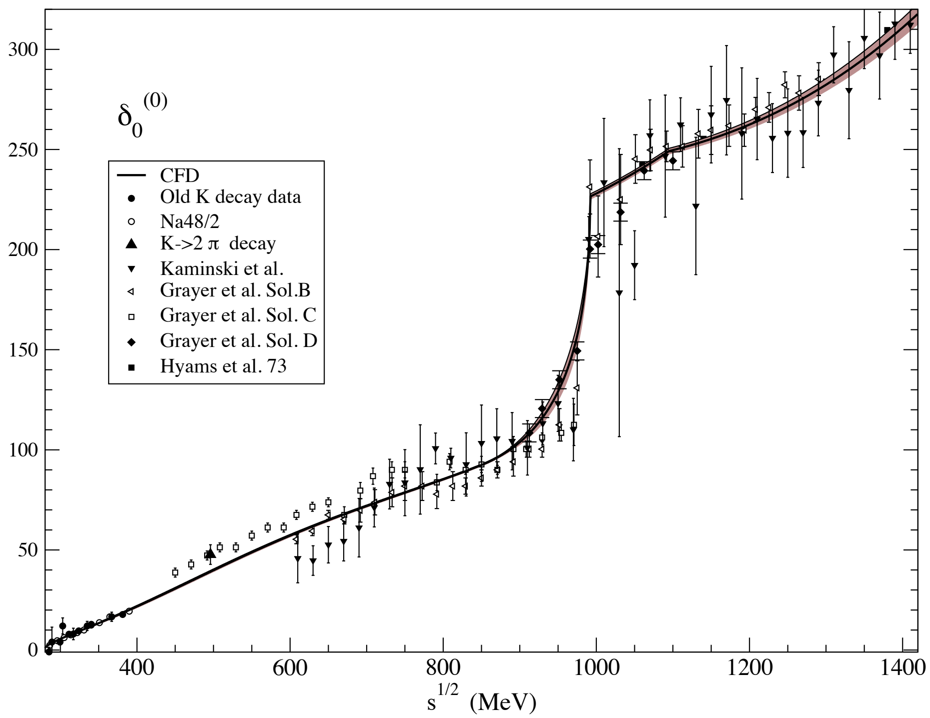
S. Geltman, *Topics in Atomic Collision Theory*, Academic Press, NY, 1969, p. 23

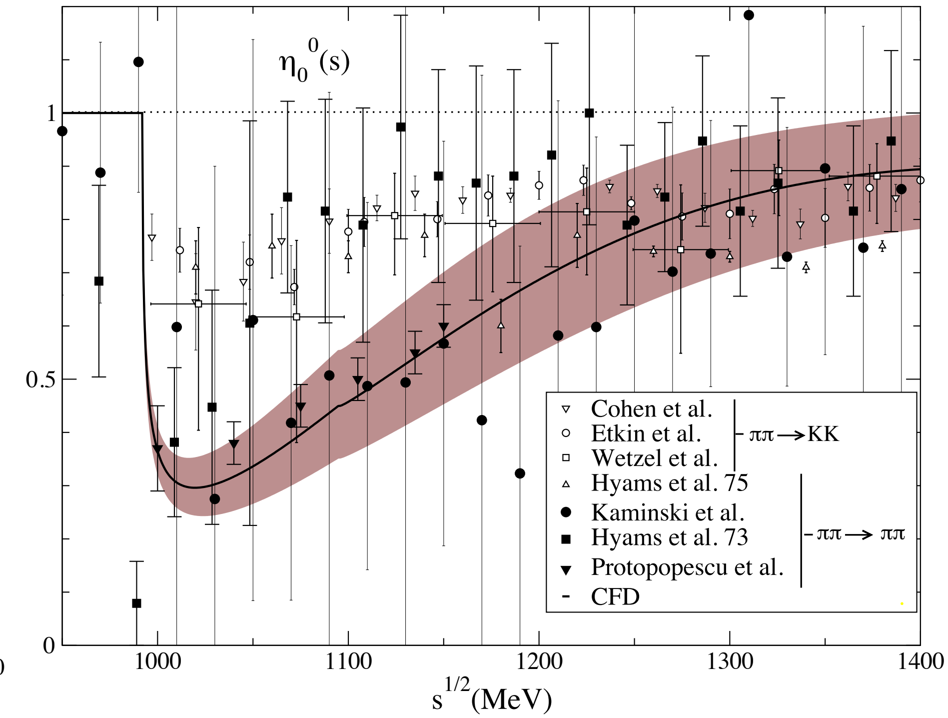
Effect is used to produce monochromatic neutron beams; $\sigma(n -{}^{56}\mathrm{Fe})$ has a dip at 24 keV, leading to transparency [P. S. Barbeau +, Nucl. Inst. Meth. A **574**, 385 (2007)]

Dip in S-wave $\pi\pi$ scattering near 1 GeV due to opening of $K\bar{K}$ threshold: S. M. Flatté *et al.*, PL **B38**, 232 (1972)

$I = 0$ PION-PION SCATTERING

R.Garcia-Martin *et al.*, Phys. Rev. D **83**, 074004 (2011):





S-wave phase shift δ_0^0 ↑ S-wave inelasticity $\eta_0^0(s)$ ↑

Here s is the square of the center-of-mass energy

Phase shift δ_0^0 goes rapidly through π just below 1 GeV and S-wave elastic $\pi\pi$ cross section vanishes there; η_0^0 dips sharply at inelastic threshold for $\pi\pi \to K\bar{K}$

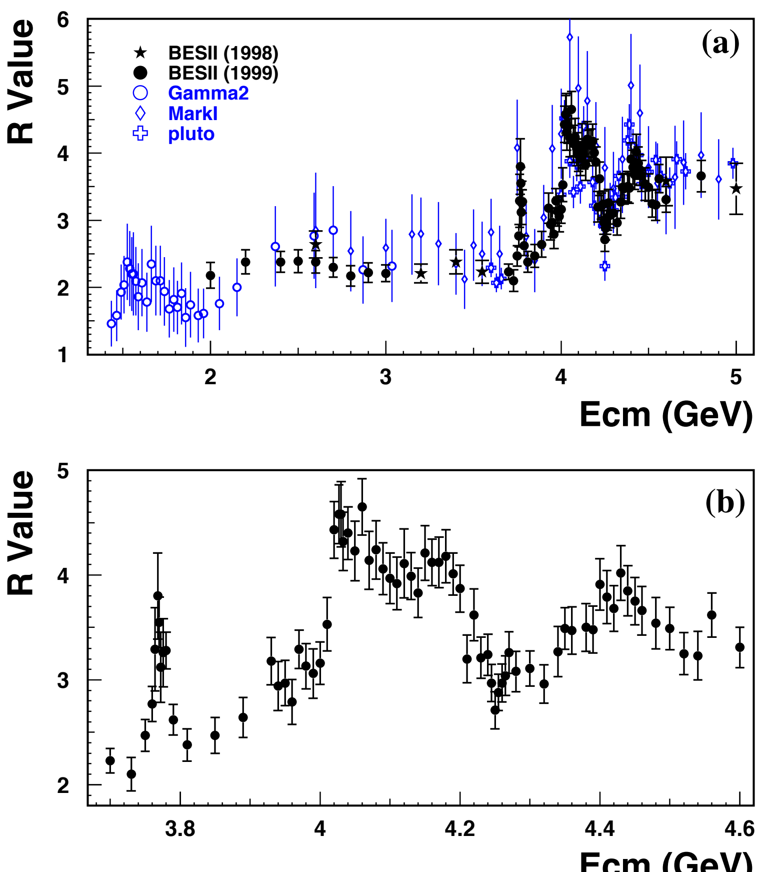
S-WAVES NEAR THRESHOLDS

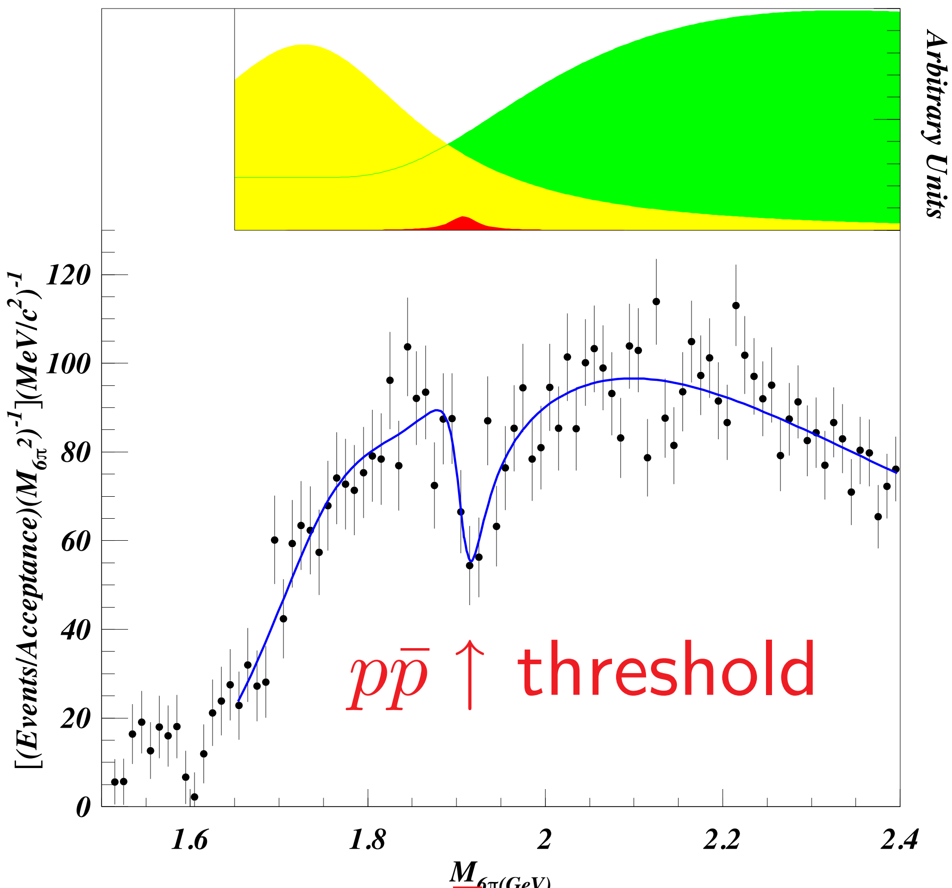
Cusps and dips: J. L. Rosner, PR D **74**, 076006 (2006)

$\pi\pi \rightarrow K\bar{K}$ only one example where new threshold is associated with a dip in the elastic cross section

$$R = \frac{\sigma(e^+e^-) \rightarrow \text{hadrons}}{\sigma(e^+e^- \rightarrow \mu^+\mu^-)}$$

$3\pi^+3\pi^-$ photoproduction





S-wave charm ↑ threshold $[D(1864)\bar{D}(2420) + \text{c.c.}]$

SCATTERING LENGTH

For small k, $\delta_\ell(k) \sim k^{2\ell+1}$ (Merzbacher, 3rd ed., p. 309)

In particular, $\delta_0 \to -ka$ as $k \to 0$; $a=$ *scattering length*

Scattering length approximation to the S-matrix:

$S = e^{2i\delta} \simeq \frac{1+i\delta}{1-i\delta} = \frac{1-ika}{1+ika} = \frac{1/a-ik}{1/a+ik}$; *pole* at $k = i/a$

Bound state at $k = i\alpha$ for $a = 1/\alpha > 0$; example is deuteron

When a is large and negative one has a *virtual state*, as in ${}^1S_0$ nucleon-nucleon scattering near threshold

Effective range r_0: the next term in an expansion $k\ \cot\ \delta = -(1/a) + (r_0 k^2/2)$

No linear term in k because $\delta(-k) = -\delta(k)$

RELATIVISTIC NORMALIZATION

Cross section in terms of invariant matrix element $\mathcal{M}_{fi}$:

$$\frac{d\sigma}{d\Omega} = \frac{1}{(8\pi)^2 s}\left(\frac{q_f}{q_i}\right)|\mathcal{M}_{fi}|^2 = |f(\Omega)|^2$$

$q_{f,i} =$ (final, initial) c.m. momenta; $s = E^2_{\rm c.m.}$

Partial waves: $f(\Omega) = \frac{1}{q_i}\sum_\ell (2\ell+1)T^\ell(s)P_\ell(\cos\theta)$

$T_\ell(s) = \frac{\eta_\ell e^{2i\delta_\ell - 1}}{2i}$ satisfies unitarity for $\eta_\ell \leq 1$

Lorentz-invariant transition amplitude: $T_{fi} = \sqrt{\rho_f}\hat{T}_{fi}\sqrt{\rho_i}$;
$\rho_{i,f} =$ 2-body phase sp. factors $2q_{i,f}/m$ ($\rightarrow 1$ as $m \rightarrow \infty$).

$\mathcal{M}_{fi} = 16\pi\hat{T}_{fi}(\Omega)$; for elastic scattering $\hat{T}^\ell = \frac{1}{\rho}e^{i\delta}\sin\delta_\ell$.

RESONANCES

In partial wave ℓ : $\sigma_\ell = (4\pi/k^2)\sin^2\delta_\ell(2\ell+1)$

When $\delta = \pi/2$, σ_ℓ is maximum

Can represent any $S_\ell(k) = e^{2i\delta_\ell} = (a-ib)/(a+ib)$

At a resonance $S_\ell = -1$ so $a = 0$, $b =$ constant

Normalization choice: $a = E - E_0$, $b = \Gamma/2$, defining Γ.

We shall see that Γ must be positive

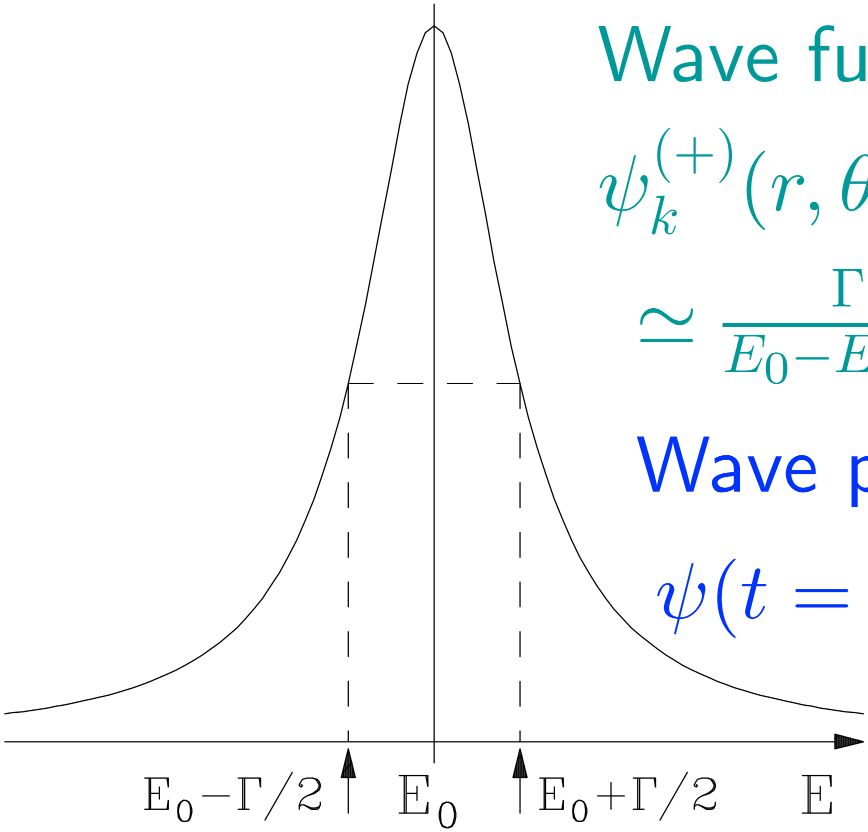
Then $S_\ell(k) = (E - E_0 - i\Gamma/2)/(E - E_0 + i\Gamma/2)$

$f_\ell(k) = \frac{S_\ell(k)-1}{2ik} = \frac{1}{2ik}\left[\frac{-i\Gamma}{E-E_0+i\Gamma/2}\right] = -\frac{\Gamma/2k}{E-E_0+i\Gamma/2}$

$\sigma_\ell(\mathrm{res}) = 4\pi(2\ell+1)|f_\ell(k)|^2 = \frac{4\pi}{k^2}(2\ell+1)\frac{\Gamma^2}{4(E-E_0)^2+\Gamma^2}$

(Breit-Wigner resonance)

BREIT-WIGNER INTERPRETATION



Wave function inside sphere of $r < a$:

$$\psi_k^{(+)}(r,\theta) \simeq e^{i\delta_\ell} \sin\delta_\ell \; g_{\ell,k}(r,\theta)$$

$\simeq \frac{\Gamma/2}{E_0 - E - i\Gamma/2} g_{\ell,k}(r,\theta)$ (g slowly varying)

Wave packet with width $\Delta E \gg \Gamma$:

$$\psi(t=0) = \int_{\Delta E} \rho(E) \frac{\Gamma/2}{E_0 - E - i\Gamma/2} g_{\ell,k}(r,\theta)$$

($\rho(E)$ peaked wt. function)

Then $\psi(t) \simeq \rho(E_0) g_{\ell,k_0}(r,\theta) \int_{\Delta E} \frac{\Gamma/2}{E_0 - E - i\Gamma/2} e^{-iEt} dE$

which can be performed for $t > 0$ by contour integration

Close contour in lower plane around $E = E_0 - i\Gamma/2$ pole

Then find $|\psi(t)/\psi(0)|^2 = e^{-\Gamma t}$ so $1/\Gamma$ is “lifetime”; $\Gamma > 0$

ABSORPTION

Had $\psi_k^{(+)}(r,\theta) = \sum_\ell \frac{a_\ell(k) P_\ell(\cos\theta)}{2ikr}[(-i)^\ell e^{ikr} e^{i\delta\ell} - i^\ell e^{-ikr} e^{-i\delta_\ell}]$

Let outgoing partial wave be attenuated by η_ℓ, $0 \leq \eta_l \leq 1$

$\psi_k^{(+)}(r,\theta) = \sum_\ell \frac{a_\ell(k) P_\ell(\cos\theta)}{2ikr}[(-i)^\ell e^{ikr} \eta_\ell e^{i\delta\ell} - i^\ell e^{-ikr} e^{-i\delta_\ell}]$

All previous derivations go through as before, but now

$f_k(\theta) = \sum_\ell P_\ell(\cos\theta)(2\ell+1) f_\ell(k)$; $\quad f_\ell(k) = \frac{[\eta_\ell e^{2i\delta_\ell} - 1]}{2ik}$

Note that if $\eta_\ell < 1$ then Im $f_\ell(k) \neq k |f_\ell(k)|^2$

Optical theorem $\sigma_T = (4\pi/k)\ \mathrm{Im} f(\theta = 0)$ still holds

Elastic cross section $\sigma_{\mathrm{el}} = \int d\Omega \frac{d\sigma}{d\Omega} = \int d\Omega\ |f_k(\theta)|^2$

$$= \sum_\ell (2\ell+1)(\pi/k^2)(\eta_\ell^2 + 1 - 2\eta_\ell \cos 2\delta_\ell)$$

and we need the *inelastic* cross section $\sigma_{\mathrm{in}} = \sigma_T - \sigma_{\mathrm{el}}$

INELASTIC CROSS SECTION

Compare $e^{\pm ikr}$ fluxes $I = \int d\vec{\sigma} \cdot \vec{j}$ ($d\vec{\sigma}$ = area element; $\vec{j}$ = probability current); find in each partial wave

$$I_{\rm in} = (2\ell + 1)\pi/mk \;; \quad I_{\rm out} = \eta_\ell^2(2\ell + 1)\pi/mk$$

so $I_{\rm in} - I_{\rm out} = \sum_\ell (\pi/mk)(2\ell + 1)(1 - \eta_\ell^2)$

Incident particles in a time interval dt sweeping out a volume V impinging on an area A: $N = v_0 dt A$, so flux per unit time per unit area is $I_0 = N/(Adt) = v_0 = k/m$

Then $\sigma_{\rm in} = \frac{I_{\rm in} - I_{\rm out}}{I_0} = \sum_\ell (2\ell + 1)(\pi/k^2)(1 - \eta_\ell^2)$

$$\sigma_T = \sigma_{\rm in} + \sigma_{\rm el} = \sum_\ell (2\ell + 1)(2\pi/k^2)(1 - \eta_\ell \cos 2\delta_\ell)$$

Im $f_\ell(k) = \frac{1 - \eta_\ell \cos 2\delta_\ell}{2k}$ so Im $f_k(0) = \sum_\ell (2\ell + 1)\frac{1 - \eta_\ell \cos 2\delta_\ell}{2k}$

which is just $k\sigma_T/(4\pi)$, proving optical theorem

OPTICAL ANALOGUES

Inelastic scattering occurs whenever $\eta_\ell < 1$

Always accompanied by elastic scattering:

$$1 + \eta_\ell^2 - 2\eta_\ell \cos 2\delta_\ell \neq 0 \text{ when } \eta_\ell < 1$$

Black disk: $\eta_\ell = 0$ for $\ell \leq kR$; $\eta_\ell = 1, \delta_\ell = 0$ for $\ell > kR$

For high energies such that $kR \gg 1$, where R is the range of scattering, can expect many partial waves to contribute, and $f_\ell(k)$ is fairly continuous in ℓ and k. It is then convenient to define the *impact parameter* $b \equiv (\ell + 1/2)/k$ and replace $\sum_\ell$ by $k\int db$.

Then for black disk $\sigma_{\rm in} = \sigma_{\rm el} = \pi R^2$, $\sigma_T = 2\pi R^2$

Define *momentum transfer* $t = -q^2 \equiv -2k^2(1 - \cos\theta)$

Will express near-forward scattering in terms of b and t

EIKONAL APPROXIMATION

Large-ℓ Legendre polynomials near forward direction:

$$P_\ell(\cos\theta) \simeq J_0[(\ell + \tfrac{1}{2})\sqrt{2(1-\cos\theta)}] = J_0(bq)$$

With $h(b,k) \equiv 1 - \eta_\ell e^{2i\delta_\ell}$ and $\sum_\ell (2\ell+1) \simeq 2\int \ell d\ell$:

$$f_k(\theta) = \sum_\ell P_\ell(\cos\theta)(2\ell+1)(\eta_\ell e^{2i\delta_\ell} - 1)/(2ik)$$

$$\simeq ik \int_0^\infty b\; db\; J_0(bq) h(b,k)$$

Black sphere: $h(b,k) = 1\ (b \le R)$; $h(b,k) = 0\ (b > R)$

$$f_k(\theta) = ik \int_0^R b\; db\; J_0(bq)$$

Now $J_0(x) = \left(\frac{1}{x}\frac{d}{dx}\right)[x J_1(x)]$

so $f_k(\theta) = \frac{ik}{q^2}\int_0^{qR} dx\; \frac{d}{dx}[x J_1(x)] = \frac{ikR}{q} J_1(qR)$

DIFFRACTIVE SCATTERING

By the optical theorem, can write $\sigma_T = (4\pi)$ Im $f_k(0) = 2\pi R^2$ in agreement with previous results

Differential cross section is a diffraction pattern:

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{k^2R^2}{q^2}[J_1(qR)]^2$$

Or for small t, $\frac{d\sigma}{d|t|} \simeq \frac{\pi R^4}{4}\left(1 + \frac{R^2 t}{4}\right)$

Totem at (7,8) TeV LHC (M. Berretti, Proc. of *Diffraction 2014*, AIP Conf. Proc. 1654 (2015) 040001): $\sigma_T(pp) \simeq (98, 102)$ mb, $\Leftrightarrow R = (1.25, 1.27)$ fm [$\sigma_{\rm el} \simeq 25$ mb]

$R^2/4 \simeq 10\ \mathrm{GeV}^{-2}$ but measured $|t|$ coeff. $\simeq 19\ \mathrm{GeV}^{-2}$

Proton has an "edge": M. M. Block +, PR D **91**, 011501; JLR, PR D **90**, 117902 (2014)

PROTON EDGE

$f_k(\theta) = ik \int_0^\infty b\, db\, J_0(qb) h(b,l); \quad J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{iz\cos\phi} d\phi$

With $b = |\vec{b}|$, $q = |\vec{q}|$, $\vec{q}\cdot\vec{b} = qb\cos\phi$, $d^2\vec{q} = b\ db\ d\phi$,

can write $\quad f_k(\theta) = \frac{ik}{2\pi} \int d^2\vec{b}\ e^{i\vec{q}\cdot\vec{b}} h(b,k)$

Then $\frac{d\sigma}{d|t|} = \frac{\pi}{k^2}\frac{d\sigma}{d\Omega} = \frac{\pi}{k^2}|f_k(\theta)|^2$; $\sigma_{\rm el} = \int d|t|\, \frac{d\sigma}{d|t|} = \frac{1}{\pi}\int d^2\vec{q}\, \frac{d\sigma}{d|t|}$

so one finds $\quad \sigma_{\rm el} = 2\pi \int bdb\ |h(b,k)|^2;$

$$\sigma_T = \frac{4\pi}{k}\ {\rm Im}\ f_k(0) = 4\pi \int bdb\ {\rm Re}\ h(b,k)$$

(M. Block, Physics Reports **436**, 71 (2006), Chapter 8)

Let $h = 1\ (b < R), \quad 0\ (R > b + \Delta)$, interpolate linearly

$\sigma_T - 2\sigma_{\rm el} = (\pi\Delta/3)(2R + \Delta) \Rightarrow \Delta \simeq 1.26$ fm at 8 TeV, near QCD string-breaking distance [JLR, PL B **385**, 293 (1996); G. Bali +, PR D **71**, 114513 (2005)]

ADDING RESONANCES

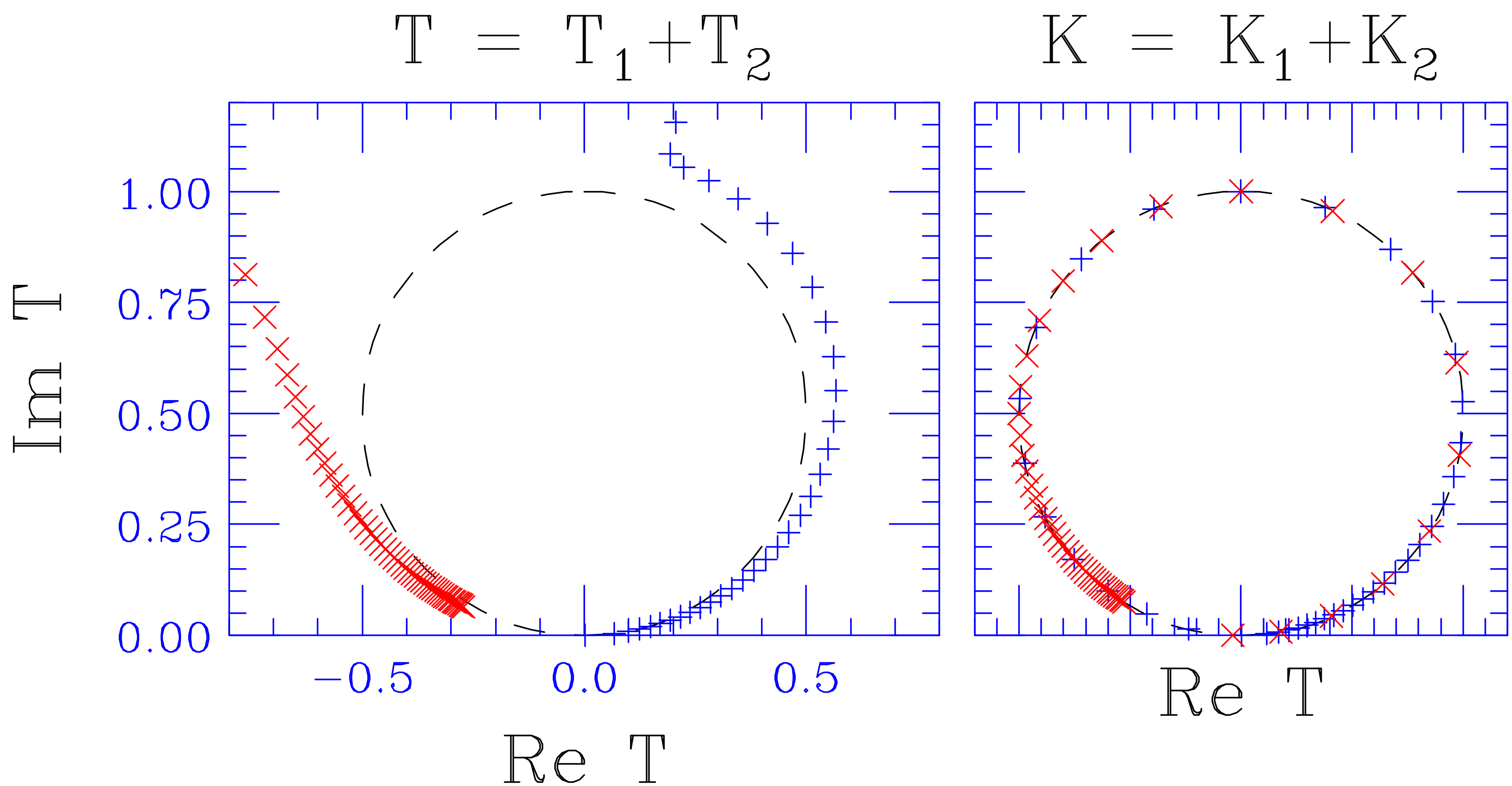
Breit-Wigner: $T(E) = e^{i\delta}\sin\delta \simeq \frac{m_0\Gamma(m)}{m_0^2 - m^2 - i m_0 \Gamma(m)}$; $\Gamma(m) = \Gamma_0 \left(\frac{\rho(m)}{\rho_0}\right) B_\ell(q(m), q_0)^2$; Γ_0, m_0 = nominal resonance width, mass; $B_\ell = \ell$-dependent barrier factor.

Corresponding K operator is $K = \frac{m_0\Gamma(m)}{m_0^2 - m^2}$, i.e., like T but without the imaginary part in the denominator. One has $T = K(\mathbb{1} - iK)^{-1} = (\mathbb{1} - iK)^{-1}K$: Interpret as a geometric series in which $(\mathbb{1} - iK)^{-1}$ describes the rescattering correction to the real operator K.

Expressing T in terms of a real K operator guarantees unitarity of S, but this is lost if $T = T_{BW,1} + T_{BW,2}$: no longer expressible in terms of a real K-matrix.

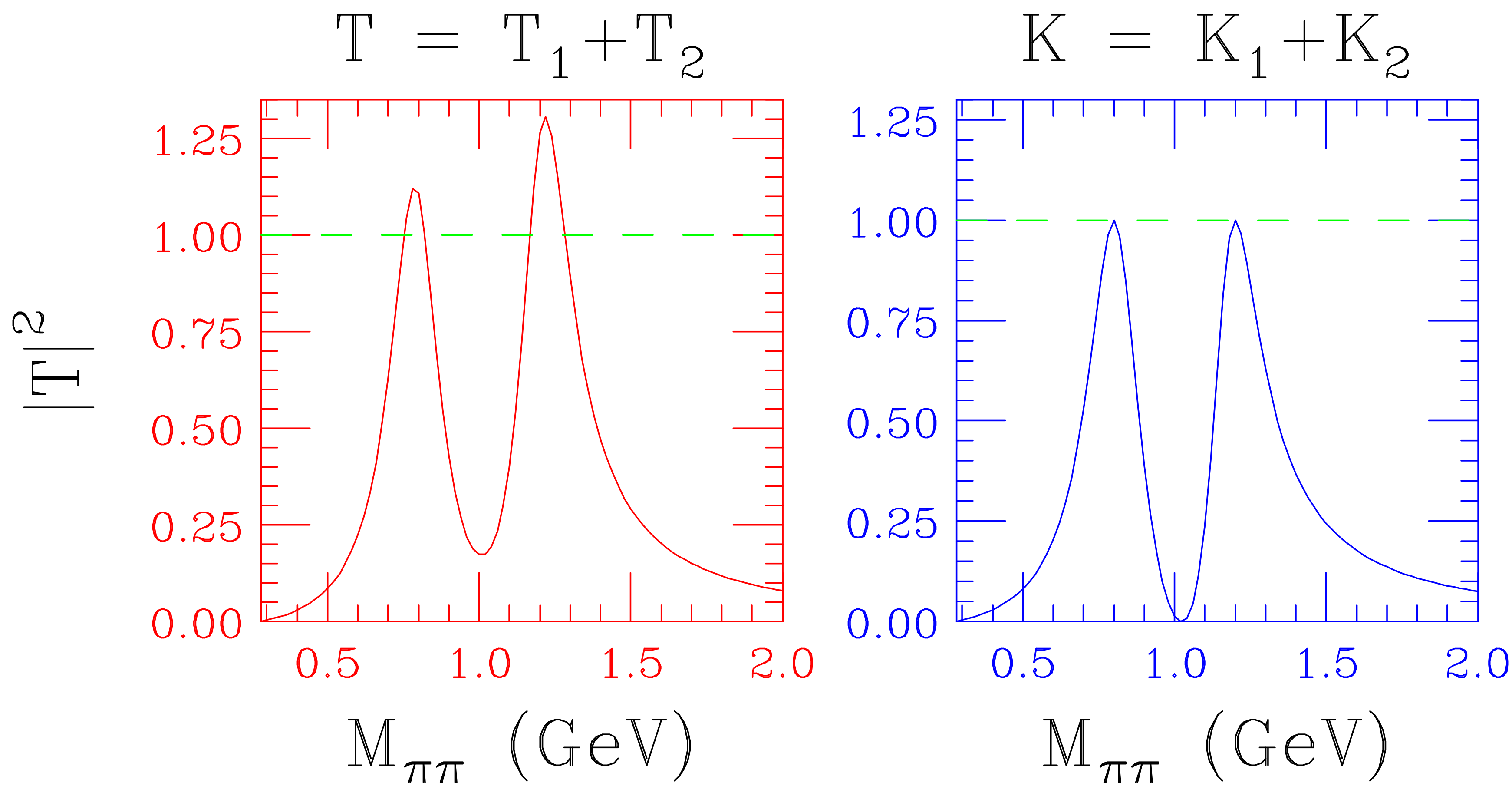
Prescription: Add Breit-Wigner resonances by adding their respective K-matrices: $K = K_{BW,1} + K_{BW,2}$.

COMPARING PRESCRIPTIONS



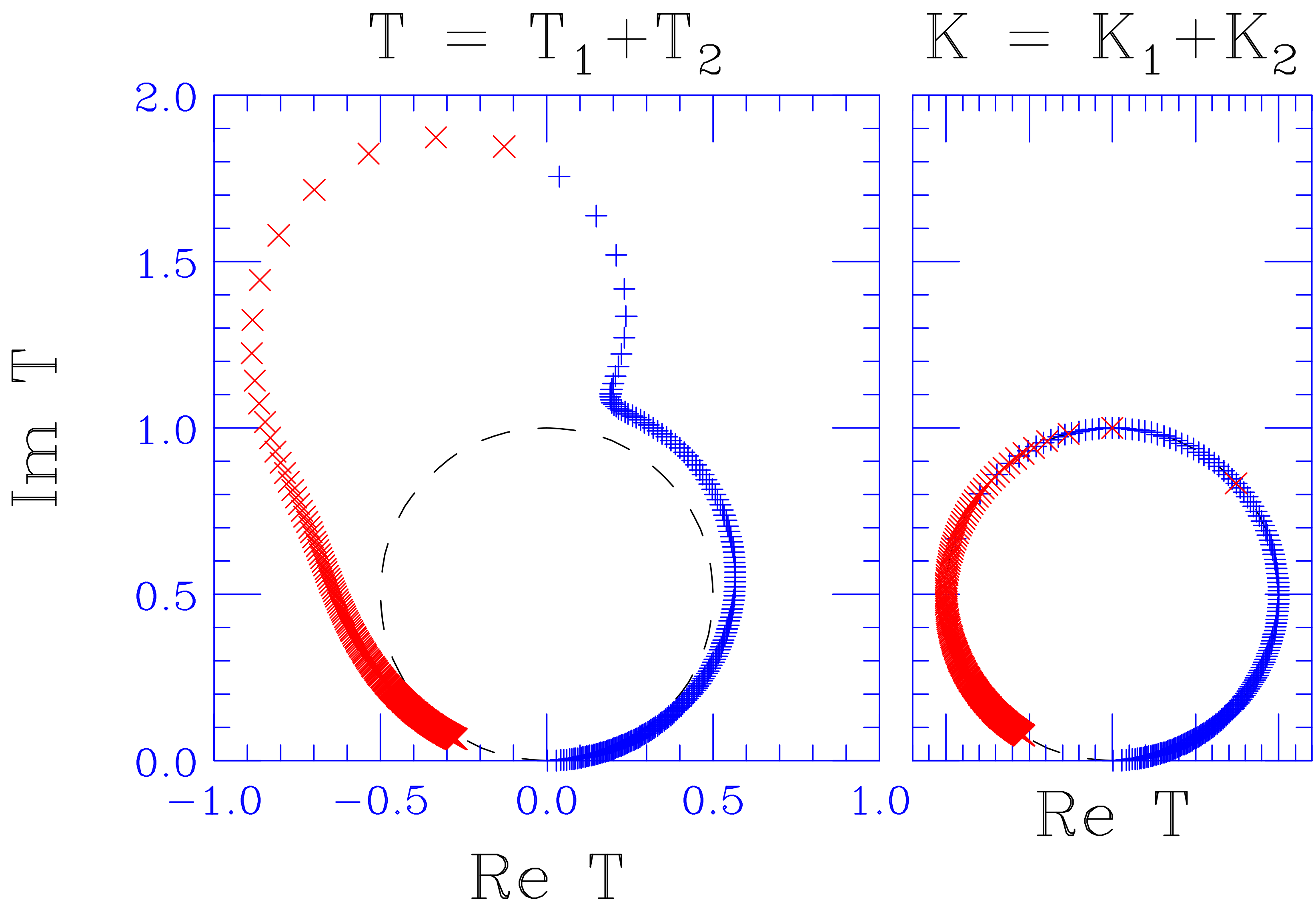
S-wave $\pi\pi$ scattering with $m_1 = 0.8$ GeV, $m_2 = 1.2$ GeV, $\Gamma_1 = \Gamma_2 = 0.2$ GeV, points every 20 MeV (blue below 1 GeV, red above 1 GeV). Adding T-matrices gives an amplitude outside unitarity circle; adding K-matrices respects unitarity.

RESONANCE SUMS: INTENSITIES



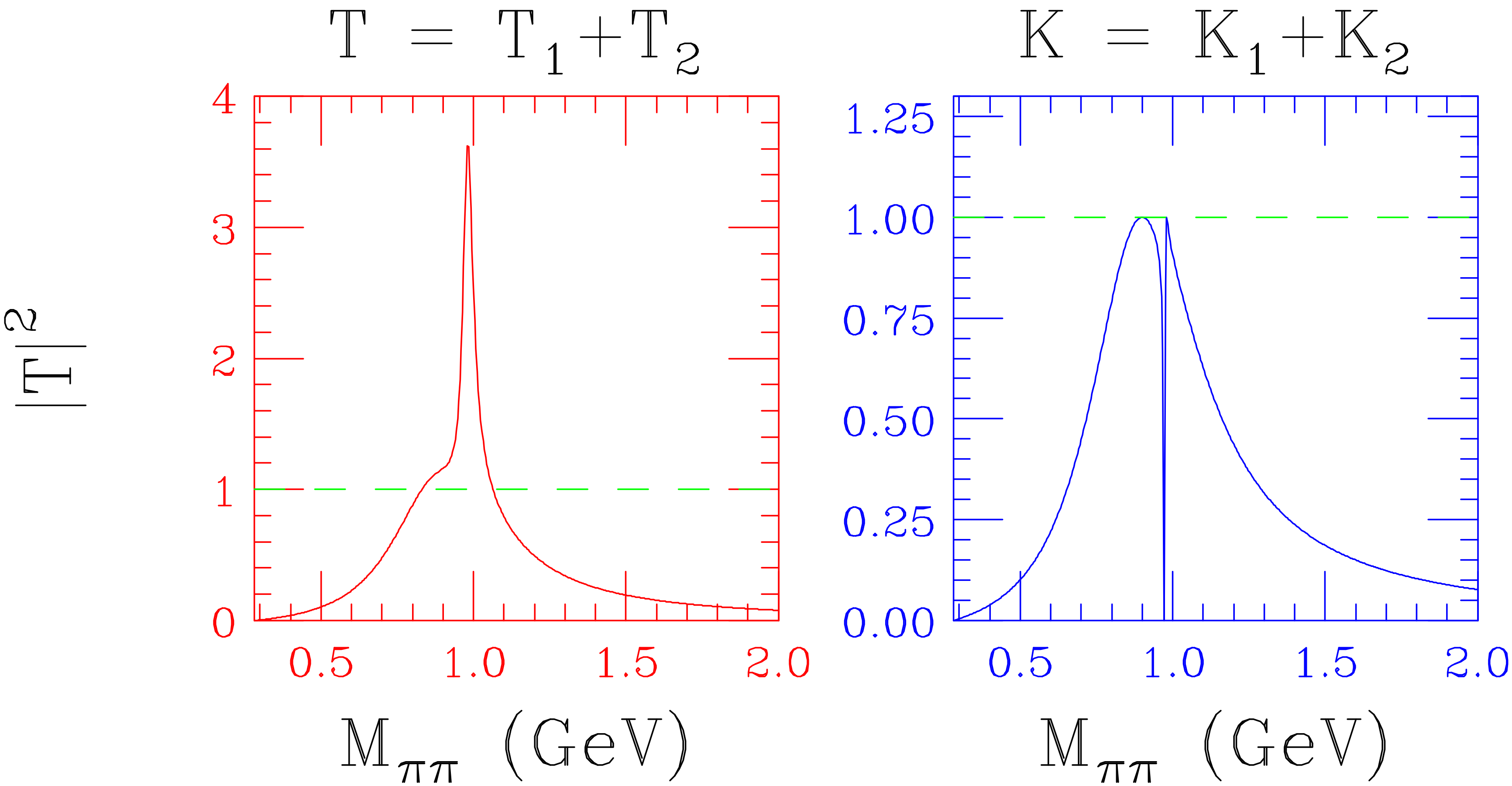
Sum of two identical resonances gives unequal peak heights (violating unitarity limit $|T|^2 \leq 1$) with $T = T_1 + T_2$ prescription. Both peaks reach the unitarity limit with $K = K_1 + K_2$ prescription.

DIFFERENT WIDTHS



$m = (0.9, 0.98)$ GeV, $\Gamma = (0.4, 0.04)$ GeV, every 4 MeV.

DIFFERENT Γ: INTENSITIES



Sum of two resonances with very different widths gives huge violation of unitarity limit $|T|^2 \leq 1$ with $T = T_1 + T_2$ prescription. Both peaks reach unitarity limit with $K = K_1 + K_2$ prescription.

DALITZ PLOT APPLICATIONS

Three-body decay $A \to B + C + D$: Describe final-state interactions (pairwise) of $B + C$, $B + D$, $C + D$.

Watson's Theorem: Final-state phase of each subsystem is that of elastic scattering in that subsystem.

This can be achieved by multiplying the "bare" matrix element for the decay by the same correction factor which converts K to a unitary amplitude: $T = K(\mathbb{1} - iK)^{-1}$ [Heitler, 1944; Dalitz, RMP **33**, 471 (1961)], so $\mathcal{M}_{fi} \to \mathcal{M}_{fi}(\mathbb{1} - iK_{BC})^{-1}(\mathbb{1} - iK_{BD})^{-1}(\mathbb{1} - iK_{CD})^{-1}$ [Aitchison, Nucl. Phys. A **189**, 417 (1972)].

This is simple as long as $B + C$, $B + D$, and $C + D$ are not "fed" by other inelastic channels, but the K-matrix should take care of them. There may also be intrinsic phases between the two-body subsystems and the bachelor particles not contained in the K-matrix formalism.

HISTORICAL NOTES

S-matrix: Heisenberg [Zeit. Phys. **120**, 513 (1943), ...].

Similar concepts utilized by Tomonaga and Dicke in microwaves (e.g., M. I. T. Radiation Laboratory Series, v. 8, Ch. 5, pp. 130-161).

Smith Chart for impedance matching [P. H Smith, Electronics **12**, 29 (1939); **17**, 130 (1944)]. Transmission line characteristic impedance: Z_0. For any impedance Z, define $z = Z/Z_0$ and $w = (z-1)/(z+1)$. Satisfies $|w| \leq 1$ since $\mathrm{Re}(z) \geq 0$. Propagation along line is just a rotation in the w-plane. This resembles transformation between K and $S = (1 - iK)/(1 + iK)$ (1 channel).

Transformation noted by Wigner in 1949; he claims to have learned it from Dicke. His R-matrix is just the K-matrix:

$$R_{ss'}(E) = \sum_\lambda \frac{\gamma_{\lambda s}\gamma_{\lambda s'}}{E_\lambda - E}$$

SUMMARY

S-matrix and its relatives (T-matrix, K-matrix, ...) have a long history in the description of scattering; S relates "in" states to "out" states

$S_\ell(k) = e^{2i\delta_\ell(k)}$ describes elastic scattering [partial wave ℓ]

Phase shifts go through $\pi/2$ at a resonance, where scattering amplitude $f_\ell(k) = (S-1)/(2ik)$ is maximal

Many interesting results follow from optical analogy;

proton is not totally black but has an "edge"

Adding resonances is best done using K-matrix, where $S = (\mathbb{1} + iK)/(\mathbb{1} - iK)$

Some simple examples given of one- and two-channel problems

S-wave behavior particlarly interesting near new thresholds

SPREADING WAVE

Expand about $\vec{q}=\vec{p}$; define $\vec{k}\equiv\vec{q}-\vec{p}$ and $v_i\equiv\partial E_p/\partial p_i$

$$E_q = E_p + \vec{k}\cdot\vec{v} + \tfrac{1}{2}k_i k_j \frac{\partial^2 E_p}{\partial p_i \partial p_j} + \ldots .$$

$$\psi_{\vec{p}}(\vec{r},t) = e^{-iE_pt}\chi_{\vec{p}}\int d^3k\ \phi(\vec{k})e^{i\vec{k}\cdot(\vec{r}-\vec{v}t)}(1-\tfrac{it}{2}k_ik_j\frac{\partial^2 E_p}{\partial p_i\partial p_j}+\ldots)$$

$$= e^{-iE_pt}\chi_{\vec{p}}(1+\frac{it}{2}\frac{\partial^2 E_p}{\partial p_i\partial p_j}\nabla_i\nabla_j+\ldots)G(\vec{r}-\vec{v}t)\ .$$

Gaussian packet: $G(r) = Ne^{-r^2/2w^2}$

$$\nabla_i\nabla_j G(\vec{r}-\vec{v}t) = \left[-\frac{\delta_{ij}}{w^2}+\frac{(r_i-v_it)(r_j-v_jt)}{(w^2)^2}\right]G(\vec{r}-\vec{v}t)\ .$$

NR: $\partial^2 E_p/(\partial p_i \partial p_j) = \delta_{ij}/m$; parameter describing spreading is $\epsilon = \frac{t}{2}\frac{\partial^2 E_p}{\partial p_i\partial p_j}\nabla_i\nabla_j G(\vec{r}-\vec{v}t) \sim \frac{t}{2mw^2} = \frac{L(\Delta k)^2}{2p}$.

EXERCISES

Consider the reflectionless many-bound-state potential in one dimension with $S = \Pi_{i=1}^{N} S_i$ and $S_i = (k + i\alpha_j)/(k - i\alpha_j)$. Calculate the difference in the phase shifts at zero and infinite momentum k: $\delta(0) - \delta(\infty)$. This is an illustration of *Levinson's Theorem* [N. Levinson, K. Danske Vidensk. Selsk. Mat-fys. Medd. **25**, No. 9 (1949); see also S.-H. Dong *et al.*, arXiv:quant-ph/9903016].

Consider transmission of a plane wave in one dimension past a square well of depth $-V_0$ and extent $-a \leq x \leq a$. This satisfies unitarity by construction, and has multiple transmission resonances. Is $K = \sum K_i$ valid?

Use a 2-channel K-matrix to describe the behavior of S-wave $\pi\pi$ scattering as energy increases through KK threshold [S. M. Flatté *et al.*, Phys. Lett. **38B**, 232 (1972); K. L. Au *et al.*, Phys. Rev. D **35**, 1633 (1987)]

ADDITIONAL REFERENCES

K. M. Watson, Phys. Rev. **95**, 228 (1954) (Theorem).

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S-matrix and networks: E. P. Wigner, Am. J. Phys. **17**, 99 (1949); J. L. Rosner, Am. J. Phys. **61**, 310 (1993).

Reflectionless 1-dim. potentials with N bound states: A. K. Grant and J. L. Rosner, JMP **35**, 2142 (1994).

K-matrix partial-wave analysis: S. U. Chung *et al.*, Ann. d. Phys. **4**, 404 (1995).

Levinson's Theorem: S.-H. Dong *et al.*, Int. J. Theor. Phys. **39**, 469 (2000) [arXiv:quant-ph/9903016].

$\pi\pi$ scattering: V. V. Anisovich & A. V. Sarantsev, Eur. Phys. J. A **16**, 229 (2003).

BAUER'S FORMULA

Expand incoming plane wave in terms of $P_\ell(\cos\theta)$:

$e^{ikr\cos\theta} = \sum_\ell c_\ell \; j_\ell(kr) P_\ell(\cos\theta)$

Let $s \equiv \cos\theta$ and take partial wave projection:

$\frac{2}{2\ell+1} c_\ell j_\ell(kr) = \int_{-1}^{1} ds \; e^{ikrs} \frac{1}{2^\ell \ell!} \frac{d^\ell}{ds^\ell} (s^2 - 1)^\ell$

(using Rodriguez' formula for the Legendre polynomial)

Integrating ℓ times by parts (surface terms $= 0$),

$c_\ell j_\ell(kr) = \frac{2\ell+1}{2^{\ell+1}\ell!} (ikr)^\ell \int_{-1}^{1} ds \; (1 - s^2)^\ell e^{ikrs}$

Using an integral representation for $j_\ell(kr)$, this is just $(2\ell + 1) i^\ell j_\ell(kr)$, i.e., $c_\ell = (2\ell + 1) i^\ell$

SMITH CHART AND QUANTUM MECHANICS

JLR, Am. J. Phys. **61** (4), 310 (1993); thanks to Dicke

Matrix method in quantum mechanics for region of constant potential $V_0 < E,\ k^2 \equiv 2m(E - V_0)$:

$$\Psi(x) \equiv \begin{bmatrix} \psi(x) \\ \psi'(x) \end{bmatrix} \;;\quad M \equiv \begin{bmatrix} 0 & 1 \\ -k^2 & 0 \end{bmatrix} \;;\quad \frac{d\Psi(x)}{dx} = M\Psi(x)$$

Shift by a: $\Psi(x + a) = \exp(Ma)\Psi(x) = T_a\Psi(x)$

where $$T_a = \begin{bmatrix} \cos ka & k^{-1} \sin ka \\ -k \sin ka & \cos ka \end{bmatrix}$$

For $E < V_0$ define $\kappa^2 \equiv 2m(V_0 - E)$; corresponding shift

operator is $$T_a = \begin{bmatrix} \cosh\ \kappa a & \kappa^{-1}\sinh\ \kappa a \\ \kappa\ \sinh\ \kappa a & \cosh\ \kappa a \end{bmatrix}$$

CIRCUIT ANALOGY

Represent local voltage V, current I with

$$\Phi = \begin{bmatrix} V \\ I \end{bmatrix} \; ; \quad \text{(series, par.) impedances } Z_{s,p} \Rightarrow \Phi' = T_{s,p}\Phi$$

with $T_{\rm series} \equiv \begin{bmatrix} 1 & -Z_s \\ 0 & 1 \end{bmatrix}$, $T_{\rm parallel} \equiv \begin{bmatrix} 1 & 0 \\ -1/Z_p & 1 \end{bmatrix}$

Traveling wave of wavelength $\lambda = 2\pi/k$ on a transmission line of characteristic impedance Z_0 : $\Phi(x{+}a) = T_{a,Z_0}\Phi(x)$

where $T_{a,Z_0} = \begin{bmatrix} \cos\ ka & iZ_0\ \sin\ ka \\ iZ_0^{-1}\sin\ ka & \cos\ ka \end{bmatrix}$

Load impedance Z_ℓ at input of transmission line (length a, characteristic impedance Z_0) connected to antenna of impedance Z_a: take unit current $I = 1$ and voltage $V = Z_a$ at antenna ($x = a$) and calculate $Z_\ell = V(x=0)/I(x=0)$

LOAD IMPEDANCE

$$\Phi(x{=}0) = \begin{bmatrix} V(x{=}0) \\ I(x{=}0) \end{bmatrix} = T^{-1}_{a,Z_0}\Phi(x=a) = T^{-1}_{a,Z_0}\begin{bmatrix} Z_a \\ 1 \end{bmatrix}$$

$$Z_\ell = V(x{=}0)/I(x{=}0) = Z_0 \frac{Z_a \cos\ ka - iZ_0 \sin\ ka}{Z_0 \cos\ ka - iZ_a \sin\ ka}$$

yielding $\quad \frac{Z_\ell - Z_0}{Z_\ell + Z_0} = e^{2ika} \frac{Z_a - Z_0}{Z_a + Z_0}$

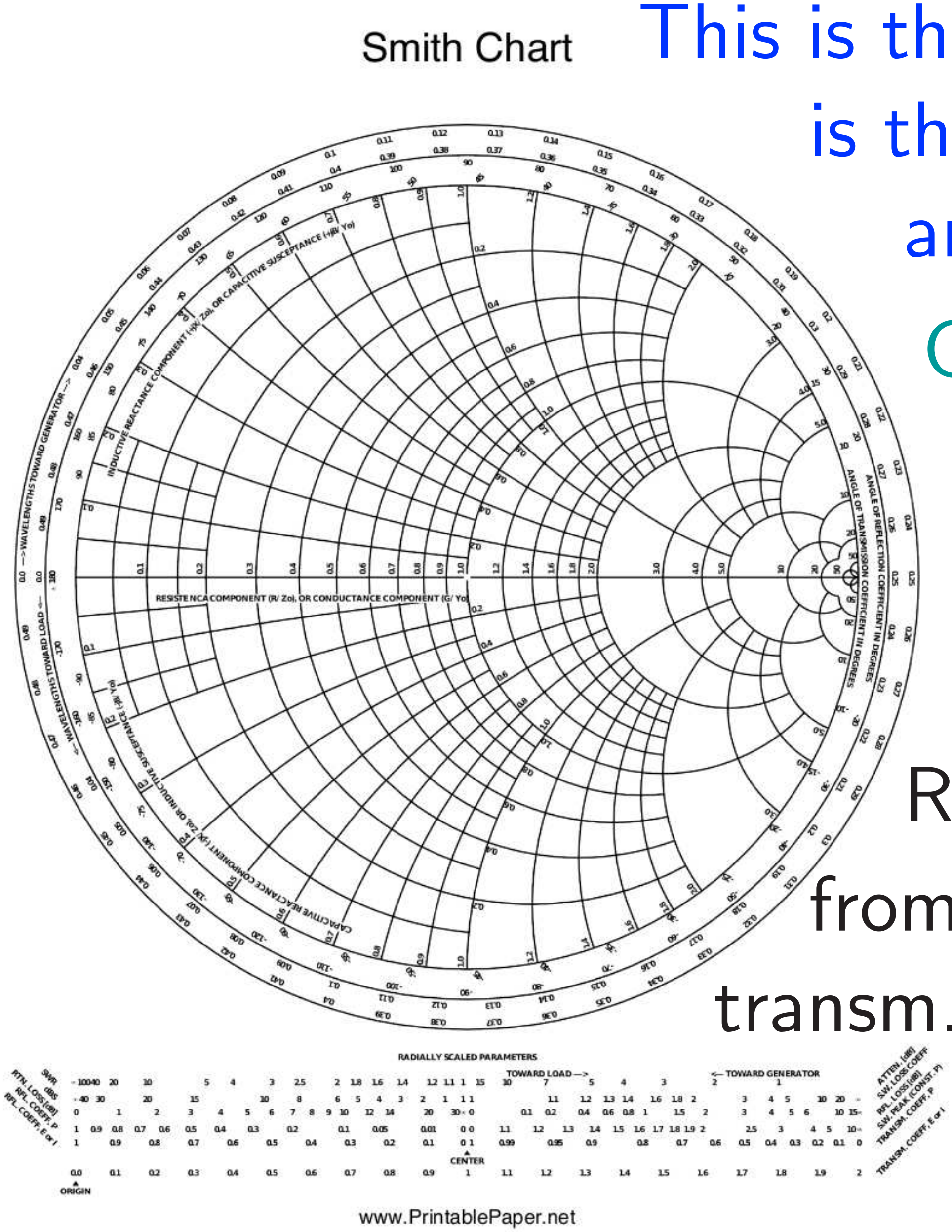
Define normalized impedance $z \equiv Z/Z_0$
and $w \equiv (z-1)/(z+1)$; then $w_\ell = e^{2ika} w_a$

$ka = 2\pi a/\lambda$ is *electric length* of transmission line

Unit circle $w = 1$: reactive impedances;
real axis $[-1 < w < 1] \Leftrightarrow$ resistances $0 < R < \infty$

Matching impedances $\Leftrightarrow$ rotations in the w plane;
wave propagation looks like effect of S-matrix

SMITH CHART



This is the $w = \frac{z-1}{z+1}$ plane; $z \equiv Z/Z_0$ is the normalized impedance and typically $Z_0 = 50\Omega$

Center corresonds to $Z{=}Z_0$

Unit circle corresponds to imaginary impedances (capacitive or reactive)

Read off complex impedances from grid; propagation along transm. line = rotation in W-plane