How to find phase shifts

Assume that $V(r)$ has finite range: $V(r) = 0$ for $r > R$.

(The method actually works provided $V(r) \propto \frac{1}{r^2}$ for large r. Note this excludes Coulomb scattering.)

We'll consider the $r > R$ and $r < R$ regions separately, then match.

First, for $r > R$,

$$\psi^+(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) P_\ell(\cos\theta) A_\ell(r),$$

where $A_\ell(r) = C_\ell j_\ell(kr) + D_\ell n_\ell(kr)$

$r=0$ not included, so these are O.K.

It's convenient to define spherical Hankel functions:

$$\begin{cases} h_\ell^{(1)}(kr) = j_\ell(kr) + i n_\ell(kr) \sim \dfrac{e^{i(kr - \ell\pi/2)}}{ikr} \\ h_\ell^{(2)}(kr) = j_\ell(kr) - i n_\ell(kr) \sim \dfrac{e^{-i(kr - \ell\pi/2)}}{ikr} \end{cases}$$

for large r

Compare to the scattering wavefunction in terms of phase shifts:

$$\psi^+(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} (2\ell+1) P_\ell(\cos\theta) \left[\frac{e^{2i\delta_\ell} e^{ikr} - e^{-i(kr - \ell\pi)}}{2ikr} \right]$$

This yields:

$$A_\ell(r) = c_\ell^{(1)} h_\ell^{(1)}(kr) + c_\ell^{(2)} h_\ell^{(2)}(kr) \quad \text{where}$$

$$c_\ell^{(1)} = \tfrac{1}{2} e^{2i\delta_\ell} \quad \text{and} \quad c_\ell^{(2)} = \tfrac{1}{2}.$$

$$\Rightarrow \boxed{A_\ell(r) = e^{i\delta_\ell}\left[\cos(\delta_\ell)\, j_\ell(kr) - \sin(\delta_\ell)\, n_\ell(kr)\right]}$$

call this $\maltese$ for later reference

Now consider the logarithmic derivative of $A_\ell(r)$, at $r = R$:

$$\beta_\ell \equiv \left.\frac{d(\ln A_\ell)}{d(\ln r)}\right|_{r=R} = \left.\frac{r}{A_\ell}\frac{dA_\ell}{dr}\right|_{r=R}$$

(Note: any constant multiplying A_ℓ cancels!)

$$\beta_\ell = kR\left[\frac{j_\ell'(kR)\cos(\delta_\ell) - n_\ell'(kR)\sin\delta_\ell}{j_\ell(kR)\cos(\delta_\ell) - n_\ell(kR)\sin\delta_\ell}\right]$$

Now solve for the phase shifts in terms of β_ℓ:

$$\boxed{\tan(\delta_\ell) = \frac{kR\, j_\ell'(kR) - \beta_\ell\, j_\ell(kR)}{kR\, n_\ell'(kR) - \beta_\ell\, n_\ell(kR)}}$$

So the problem reduces to finding the β_ℓ's.

This we do by noting that the β_ℓ's are continuous, so

$$\beta_\ell \Big|_{r>R \text{ (outside)}} = \beta_\ell\Big|_{r<R \text{ (inside)}}$$

To get the inside solution, let $u_\ell = r A_\ell$, plug $\psi^+(r)$ into Schrodinger's equation. That tells us:

$$\frac{d^2}{dr^2}u_\ell + \left(k^2 - \frac{2m}{\hbar^2}V(r) - \frac{\ell(\ell+1)}{r^2}\right)u_\ell = 0$$

So one strategy to get $\frac{d\sigma}{d\Omega}$ is:

1) Solve for u_ℓ (or A_ℓ) in the regim $(r<R)$.
   Might be very hard, possibly done numerically.
2) Use resulting $A_\ell = u_\ell/r$ to get $\beta_\ell \equiv \frac{r}{A_\ell}\frac{dA_\ell}{dr}\Big|_{r=R}$.
3) Plug into boxed formula to get $\tan(\delta_\ell)$.
4) Use $f(\vec{k},\vec{k}') = f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos\theta)$.

Example Hard-sphere scattering

$$V(r) = \begin{cases} 0 & \text{for } r>R \\ \infty & \text{for } r<R \end{cases}$$

(this is the QM analog of the classical ping-pong ball scattering from a bowling ball.)

This example is nice because the solution for $r<R$ is trivial:

$$\psi^+(r) = 0 \Rightarrow A_\ell(r)\Big|_{r=R} = 0.$$

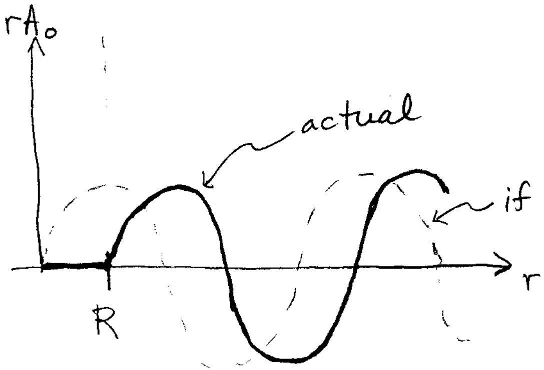
Therefore, $\cos(\delta_\ell)\, j_\ell(kR) - \sin(\delta_\ell)\, n_\ell(kR) = 0$ (from ☆ on p. 102 of these notes).

So $\boxed{\tan(\delta_\ell) = \dfrac{j_\ell(kR)}{n_\ell(kR)}}$ for each ℓ.

This is especially simple for S-wave $(\ell = 0)$ scattering.

$$\tan(\delta_0) = \frac{\frac{\sin(kR)}{kR}}{\frac{-\cos(kR)}{kR}} = -\tan(kR) \quad \Rightarrow \quad \delta_0 = -kR$$

$$\text{So } A_{\ell=0} \propto \frac{\sin(kr)}{kr}\cos(\delta_0) + \frac{\cos(kr)}{kr}\sin(\delta_0) = \frac{1}{kr}\sin(kr + \delta_0)$$
$$= \frac{1}{kr}\sin(k(r-R))$$



The wave is just shifted out by R.

What about the low-energy limit (long wavelengths)?

Then $kR \ll 1$, and

$$j_\ell(kR) \simeq \frac{(kR)^\ell}{\underbrace{(1)(3)(5)\ldots(2\ell+1)}_{\equiv (2\ell+1)!!}} \quad \text{and} \quad n_\ell(kR) \simeq -\frac{\overbrace{(1)(3)(5)\ldots(2\ell-1)}^{\equiv (2\ell-1)!!}}{(kR)^{\ell+1}}$$

So $$\tan(\delta_\ell) = \frac{-(kR)^{2\ell+1}}{[(2\ell-1)!!]^2\,(2\ell+1)}$$ ← smaller for larger ℓ.

So keep only $\ell = 0$:

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2(\delta_0)}{k^2} = \frac{\sin^2(kR)}{k^2} \approx R^2 \quad \text{for } kR \ll 1.$$

This is <u>isotropic</u> (constant in both ϕ and $\cos(\theta)$).

Also $\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi R^2 = 4$ (classical result).

[A general fact (valid beyond this example):

At low energies, $\delta_\ell \propto k^{2\ell+1} \propto E^{\ell+1/2}$.

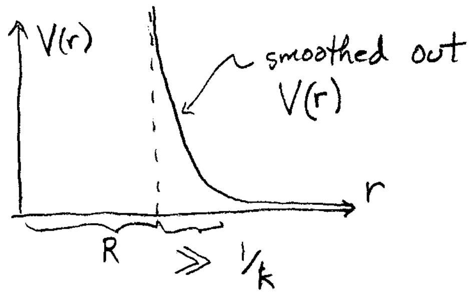
So, for small E, $\ell=0$ dominates $\Rightarrow$ mostly S-wave.

As you raise E, P-wave becomes more important, etc.]

<u>High-energy limit of hard-sphere scattering:</u>

Many δ_ℓ contribute. Can show (see Sakurai p. 408-410) that $\sigma_{tot} \simeq 2\pi R^2$ (as $k \to \infty$). This is still twice as big as the classical result; the reason is that $V(r)$ is discontinuous at $r=R$, so varies sharply on length scales shorter than the wavelength of the particles, no matter how big E is.

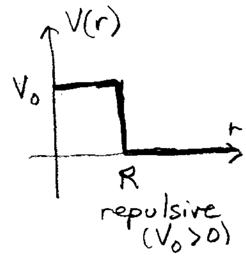
To get classical $\sigma_{tot} = \pi R^2$, need:

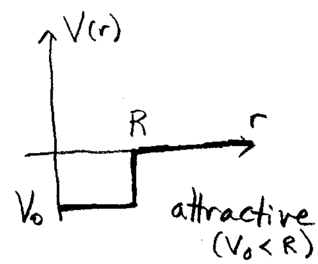


Hard-sphere scattering isn't very realistic, so consider instead...

<u>Finite well or barrier</u>

$$V = \begin{cases} V_0 & (r<R) \\ 0 & (r>R) \end{cases}$$





Only consider S-wave (valid at low E).

First consider the inside wavefunction: $\psi^+(r) \propto j_0(k'r) \propto \frac{\sin(k'r)}{k'r} \propto A_0$

where $\frac{\hbar^2 k'^2}{2m} = E - V_0$.

Outside, $\psi^+(r) \propto e^{i\delta_0}\left[j_0(kr)\cos\delta_0 - n_0(kr)\sin(\delta_0)\right] = e^{i\delta_0}\frac{\sin(kr+\delta_0)}{kr}$,

from eq. ✡ on page 102 of these notes.

Note that for an attractive potential, $k' > k$
" " " " repulsive ", $k' < k$.

Now compute $\beta_0 = \frac{r}{A_0}\frac{dA_0}{dr}\Big|_{r=R}$ (inside)

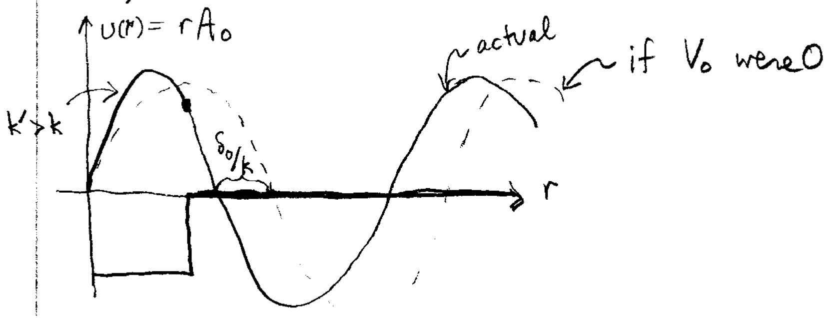
$$= \frac{r}{\left(\frac{\sin(k'r)}{k'r}\right)} \frac{d}{dr}\left(\frac{\sin(k'r)}{k'r}\right)\Bigg|_{r=R} = k'R\cot(k'R) - 1 .$$

Now plug into $\tan(\delta_0) = \dfrac{kR\, j_0'(kR) - \beta_0 j_0(kR)}{kR\, n_0'(kR) - \beta_0 n_0(kR)}$

$$= \frac{\cos(kR)\sin(k'R) - \frac{k'}{k}\cos(k'R)\sin(kR)}{\sin(kR)\sin(k'R) + \frac{k'}{k}\cos(k'R)\cos(kR)}$$ (after some algebra).

It's instructive to consider the wavefunction graphically.

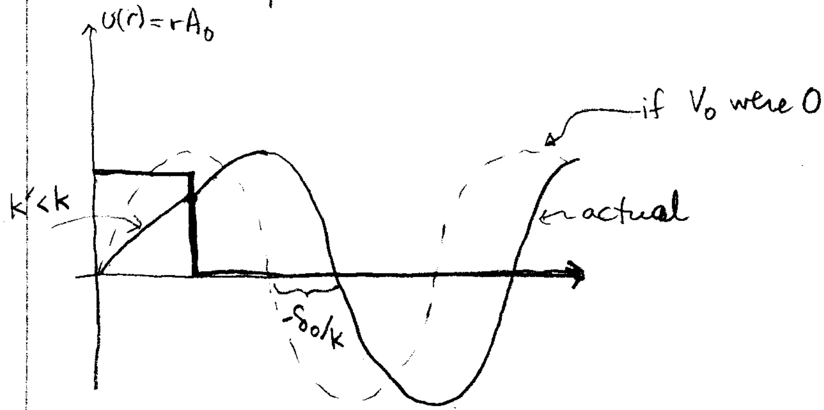
First, the attractive case:



$\underline{\delta_0 > 0 \text{ for } V_0 < 0}$

The attractive potential "pulls in" the $l=0$ wave by δ_0/k.

Now the repulsive case:



$\delta_0 < 0$ for $V_0 > 0$.

The repulsive potential "pushes out" the $l=0$ wave by $|\delta_0|/k$.

These pictures explain why δ_ℓ is called a "phase shift."

The calculation of δ_0 above works only if $E > V_0$.
Otherwise, use instead $A_0 = \frac{\sinh(\kappa R)}{\kappa R}$ for $r<R$, where
$\frac{\hbar^2\kappa^2}{2m} = V_0 - E > 0$. (You'll do this for homework.)

Now let's specialize to the attractive case $V_0 < 0$ (more common in the real world).
For small $|V_0|$, δ_0 is small.
If we increase $|V_0|$, δ_0 increases until it reaches $\delta_0 = \pi/2$.
Then the S-wave cross-section is maximal:

$$\sigma_{l=0}\Big|_{max} = \frac{4\pi}{k^2}\sin^2\delta_0 \rightarrow \frac{4\pi}{k^2} = \frac{2\pi\hbar^2}{mE}$$ is the maximum allowed.

("Saturates the partial wave unitarity bound.")
But if we keep increasing $|V_0|$, eventually $\delta_0 = \pi$, and
then $\sigma_{l=0}\Big|_{min} = \frac{4\pi}{k^2}\sin^2(\pi) = 0$.

Ramsauer-Towsend effect: no scattering even though $V(r)$ is attractive. (Actually occurs for electron scattering from noble gas atoms Ar, Kr, Xe.)

In general, for very low energy scattering ($k \to 0$ and $E \to 0$),
$\tan(\delta_0) \to -ka$ where a is called the scattering length.
Sakurai p. 413-415 gives a general argument, but let's see how this works in our previous example of a finite well:

We found $$\tan(\delta_0) = \frac{\cos(kR)\sin(k'R) - \frac{k'}{k}\cos(k'R)\sin(kR)}{\sin(kR)\sin(k'R) + \frac{k'}{k}\cos(k'R)\cos(kR)}$$

Now take $k \to 0$ (but leave $k' = \frac{\sqrt{2m(E-V_0)}}{\hbar^2}$ alone; may not be small).

Use $\sin(x) = x - \frac{x^3}{6} + \frac{x^5}{120} + \ldots$, $\cos(x) = 1 - \frac{x^2}{2} + \frac{x^4}{24} + \ldots$ for small x.

Then $\tan(\delta_0) = k\left(-R + \frac{\tan(k'R)}{k'}\right) + \mathcal{O}(k^3)$

So approximate $k' = \sqrt{\frac{-2mV_0}{\hbar^2}} = \sqrt{\frac{2m|V_0|}{\hbar^2}}$ = constant, and we get

$$a = \text{scattering length} = R - \frac{\tan(k'R)}{k'}.$$

By tuning $k'R$ just right $\approx \pi/2$ + a little bit, one can arrange for $a \gg R$. This happens if there is an S-wave bound state with small binding energy.

In general, if $\tan(\delta_0) = -ka$ for small k, and $a \gg R$, then $E_{\text{bound-state}} = -E_{\text{binding-energy}} \simeq \frac{-\hbar^2}{2ma^2}$.

Also $\sigma = \frac{4\pi}{k^2}\sin^2(\delta_0) = \frac{4\pi}{k^2}\frac{\tan^2(\delta_0)}{1+\tan^2(\delta_0)} = \frac{4\pi}{k^2}\left(\frac{k^2a^2}{1+k^2a^2}\right) = \frac{4\pi a^2}{1+k^2a^2}$

For very small ka, $\sigma \approx 4\pi a^2$.

For slightly larger ka, we can write: $\sigma = \frac{2\pi\hbar^2/m}{E - E_{\text{bound}}}$.

Note that $E > 0$ is the physical region, and $E_{\text{bound}} < 0$, so the denominator never actually blows up. But the form of this for low E indicates the presence of a bound state.

A famous case where this (doesn't quite) work is neutron-proton scattering. $np \to np$. (masses $\approx$ 938.3, 939.6 MeV/c^2)

Experimentally, for scattering with parallel spins $(S = 1)$,

$\sigma(np \to np) = 4\pi a^2$, where $a = 5.4 \times 10^{-13}$ cm

So predict a ${}^{2S+1}L_J = {}^3S_1$ bound state with energy...

$$E_{\substack{\text{bound,}\\ \text{predicted}}} = \frac{-\hbar^2}{2\underbrace{\left(\frac{m_n+m_p}{2}\right)}_{\text{reduced mass of } n,p \text{ system}} a^2} = \frac{-\hbar^2}{m_p a^2} \approx -1.4 \text{ MeV}$$

The deuteron has $E_{bound} = -E_{binding} = -2.22$ MeV, ${}^{2S+1}L_J = {}^3S_1$.

The mismatch is because we've neglected spin effects.

There is also a parallel spins $(S=0)$ scattering amplitude given by (experimentally):

$$\sigma(np \to np) = \frac{2\pi\hbar^2/m}{E - E_V} \quad \text{where } E_V \simeq -0.1 \text{ MeV}.$$

However, there is no ${}^1S_0$ bound state with $E_{bound} = -E_{binding} = -0.1$ MeV.

One says there is a "virtual bound state" with $E_{binding} = 0.1$ MeV.

(For homework, find the corresponding scattering length.)

After averaging over all spins,

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4}\frac{d\sigma}{d\Omega}\bigg|_{s=0} + \frac{3}{4}\frac{d\sigma}{d\Omega}\bigg|_{s=1}\right) = \frac{\pi\hbar^2}{2m}\left(\underbrace{\frac{1}{E+0.1 \text{ MeV}}}_{{}^1S_0 \text{ virtual bound state}} + \underbrace{\frac{3}{E+1.4 \text{ MeV}}}_{{}^3S_0 \text{ "deuteron"}}\right)$$

at low energies.

Bound states as poles in the scattering amplitude

Recall: $S_\ell(k) = e^{2i\delta_\ell}$. For $\ell = 0$,

$$\psi^+(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\frac{1}{2ik}\left[\underbrace{(1+2ikf_0)}_{S_0(k)} e^{ikr} - e^{-ikr}\right]/r$$

Now if there is a bound state with negative $E = \frac{\hbar^2 (iK)^2}{2m}$,

then $\psi_b(\vec{r}) = N e^{-Kr}/r$.

Since $\psi^+(\vec{r})$ and $\psi_b(\vec{r})$ satisfy the same Schrodinger equation,

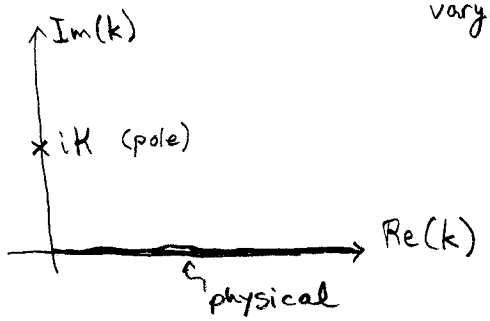
we expect $\psi_b(\vec{r}) = \psi^+(\vec{r})\Big|_{k=iK}$, up to normalization.

So, $\dfrac{e^{-Kr}}{r} \propto \dfrac{1}{r}\left[S_\ell(k)\, e^{ikr} - e^{-ikr}\right]\Big|_{k=iK} \propto \dfrac{1}{r}\left[e^{-Kr} - \dfrac{e^{+Kr}}{S_\ell(iK)}\right]$

The $\dfrac{e^{Kr}}{r}$ can't be tolerated in a bound state, so we must have $S_\ell(k) \to \infty$ as $k \to iK$.

Therefore, $S_\ell(k) = \dfrac{(\text{finite function of } k)}{k - iK}$ (pole at $k = iK$)

k varying, iK constant determined by bound state.



Also, $|S_\ell(k)| = 1$ for real positive k.

$S_\ell(0) = 1$ ($e^{2i\delta_0} \to 1$ at small E).

One can sometimes reconstruct $S_\ell(k)$ as a function of complex k, even though only real k is physical.

The poles of $S_\ell(k)$ $\leftrightarrow$ bound states.

<u>Resonant Scattering</u> Recall: $\sigma_\ell = \dfrac{4\pi}{k^2}(2\ell+1)\sin^2(\delta_\ell) = \dfrac{4\pi}{k^2}\dfrac{(2\ell+1)}{1+\cot^2(\delta_\ell)}$

Usually, $\cot^2(\delta_\ell) \gg 1$. But, if it happens that $\cot(\delta_\ell) \approx 0$, then σ_ℓ will have a maximum peak at that E.

Let's expand $\cot(\delta_\ell)$ around the value E_r where $\cot(\delta_\ell) = 0$.

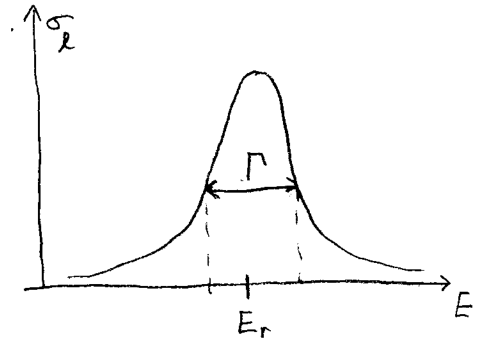
$$\cot(\delta_\ell) = \underbrace{\cot(\delta_\ell)\Big|_{E=E_r}}_{\substack{=0 \text{ by} \\ \text{assumption}}} + (E - E_r)\underbrace{\left(\frac{d\cot(\delta_\ell)}{dE}\right)\Bigg|_{E=E_r}}_{\substack{\text{call this} \\ \text{constant } \frac{2}{\Gamma}}} + \mathcal{O}\left((E-E_r)^2\right)$$

, where Γ has units of energy

$$\simeq \frac{2}{\Gamma}(E - E_r)$$

Now plug this into $\sigma_\ell = \dfrac{4\pi}{k^2}\dfrac{(2\ell+1)}{1 + \frac{4}{\Gamma^2}(E-E_r)^2}$, or, rewriting...

$$\sigma_\ell = \frac{4\pi(2\ell+1)}{k^2}\frac{\Gamma^2/4}{(E-E_r)^2+\Gamma^2/4} \quad = \text{Breit-Wigner resonance formula.}$$



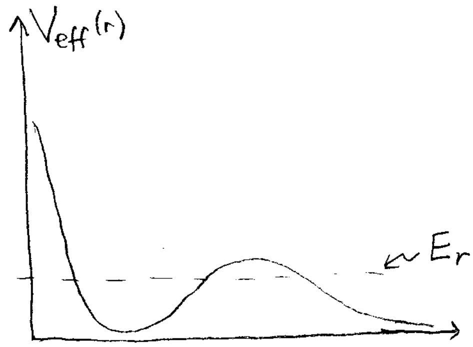
Γ = full width at half-maximum

E_r = energy of a quasi-bound state with angular momentum ℓ. (usually $\ell \geq 1$).

A quasi-bound state arises if there is a barrier in

$$V_{eff}(r) = V(r) + \frac{\hbar^2}{2m}\left[\frac{\ell(\ell+1)}{r^2}\right] \leftarrow \text{repulsive (positive and falling)}$$

which governs the effective 1-d Schrodinger equation for $A_\ell(r)$.

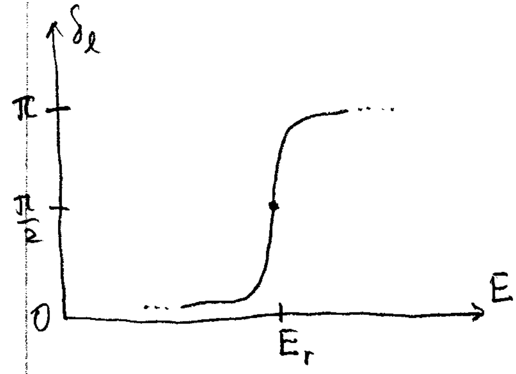


$\leftarrow E_r$ = quasi-bound state energy level

If the barrier has finite height, this is not a true bound state; a wavefunction peaked inside will always leak out, by tunneling through the barrier.

Near $E = E_r$, the phase shift behaves like:

$$\delta_\ell \simeq \frac{\pi}{2} + \tan^{-1}\left(\frac{E-E_r}{\Gamma/2}\right) \quad \text{or more generally:} \quad \delta_\ell = (n+\tfrac{1}{2})\pi + \tan^{-1}\left(\frac{E-E_r}{\Gamma/2}\right)$$

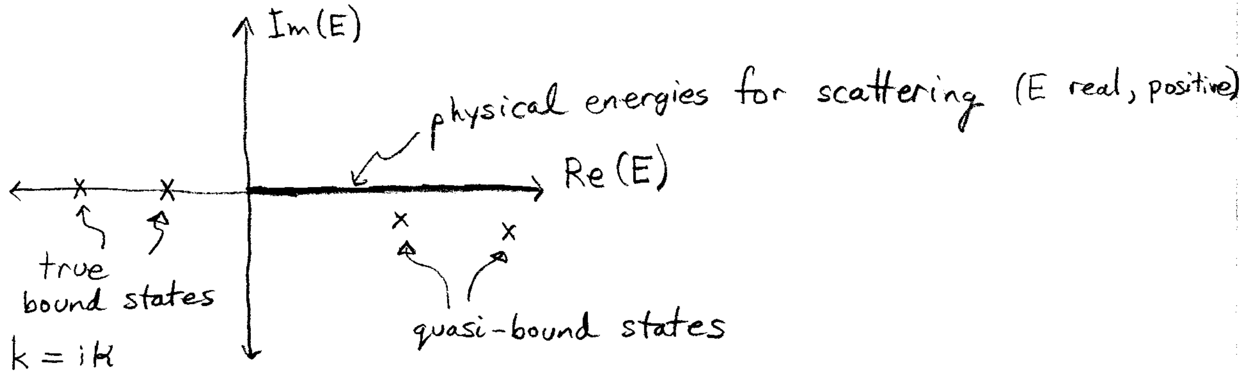


The phase shift rises through $\pi(n+\frac{1}{2})$ near a resonant energy.

Resonances also correspond to poles in the scattering amplitude:

$$S_\ell(k) = e^{2i\delta_\ell} - 1 = \frac{-i\Gamma}{E - E_r + i\Gamma/2} \implies \text{pole at } E = E_r - i\frac{\Gamma}{2}$$

In the complex energy plane, we can map two kinds of poles for $S_\ell(E)$:



$k = i\kappa$

$\Rightarrow E = -\frac{\hbar^2\kappa^2}{2m}$

Scattering of Identical Particles

So far we've neglected the possibility that the scattering particle might be identical to the particle it scatters from.

First consider two identical bosons with no spin (for example, α's).

The total wavefunction $\Psi(\vec{r}_1, \vec{r}_2) = e^{i\vec{P}\cdot(\vec{r}_1+\vec{r}_2)}\,\psi(\vec{r})$ $\quad \vec{r} = \vec{r}_1 - \vec{r}_2$

must be symmetric under $\vec{r}_1 \leftrightarrow \vec{r}_2$.

So $\psi(\vec{r}) = \psi(-\vec{r})$ for the relative wavefunction.

(Recall this means even parity.)

If we neglected the symmetry, we would have $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(\theta)\frac{e^{ikr}}{r}$.

The correct wave function must be instead:

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\vec{r}} + [f(\theta) + f(\pi-\theta)]\,\frac{e^{ikr}}{r} \qquad \text{(in COM frame)}$$

So $$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi-\theta)|^2 = |f(\theta)|^2 + |f(\pi-\theta)|^2 + 2\,\mathrm{Re}[f^*(\theta)\,f(\pi-\theta)].$$