6 Scattering Theory

Scattering processes: continuum initial state
$\downarrow$
continuum final state

} important experimental tool

⇝ difference between initial and final state tells us about potential

6.1: Scattering as a time-dependent perturbation

Consider $\hat{H} = \underbrace{\frac{\hat{\vec{p}}^2}{2m}}_{\hat{H}_0} + V(\vec{x})$ time-independent

↪ eigen energies $E_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$

plane wave eigenkets $|\vec{k}\rangle$

Idea in this section: Incoming particle will "see" the scattering potential as a perturbation that is "turned on" only during the time that the particle is in vicinity of scatterer.

A word of caution: In general, the scattering potential will have non-perturbative effect!

Here: Let's apply the time-dependent perturbation theory framework to time-independent problem.
→ use interaction picture.

Short review:

$$|\alpha, t; t_0\rangle_I = \hat{U}_I(t, t_0)\,|\alpha, t_0; t_0\rangle_I$$

$$i\hbar \frac{\partial}{\partial t} \hat{U}_I(t, t_0) = \hat{V}_I(t)\,\hat{U}_I(t, t_0)$$

$$\hat{V}_I(t) = e^{i\hat{H}_0 t/\hbar}\,\hat{V}\,e^{-i\hat{H}_0 t/\hbar}$$

$$\hat{U}_I(t_0, t_0) = \hat{\mathbb{1}}$$

$$\hat{U}_I(t, t_0) = \hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\,\hat{U}_I(t', t_0)\,dt'$$

Let $|i\rangle$ and $|n\rangle$ be eigen~~kets~~ of $\hat{H}_0$. Transition amplitude:

$$\boxed{\langle n|\hat{U}_I(t, t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar}\sum_m \langle n|\hat{V}|m\rangle \int_{t_0}^{t} e^{i\omega_{nm}t'}\langle m|\hat{U}_I(t', t_0)|i\rangle\,dt'}$$

where $\hbar\omega_{nm} = E_n - E_m$

So far, I just rewrote the equations we had in the context of time-dep. PT.

Plane wave initial and final states:

"Box normalization"

$\vec{k}$: discrete values

when $L \to \infty$, k becomes continuous variable

$$\langle \vec{x}, \vec{k} \rangle = \frac{1}{L^{3/2}} e^{i \vec{x} \cdot \vec{k}}$$

$$\langle \vec{k}', \vec{k} \rangle = \delta_{\vec{k}' \vec{k}}$$

$\vec{k}$ takes discrete values

$L \to \infty$ at end of calculation (we assume that the system lives in a big box)

We want $\underbrace{t \to \infty \text{ and } t_0 \to -\infty}$.

recall, we are dealing with a time-independent problem

Write out transition amplitude in first-order PT, i.e., replace $\hat{U}_I$ in integrand by $\mathbb{1}$:

$$\langle n | \hat{U}_I(t, t_0) | i \rangle = \delta_{ni} - \frac{i}{\hbar} \langle n | \hat{V} | i \rangle \int_{t_0}^{t} e^{i \omega_{ni} t'} dt'$$

how to let $t \to \infty$ and $t_0 \to -\infty$?

We now define a T-matrix through the matrix elements T_{ni}. The definition may appear a bit arbitrary... We will see below that the T- and S-matrix are related to the scattering cross section.

The equation that defines T_{ni} reads:

$$\langle n | \hat{U}_I(t, t_0) | i \rangle = S_{ni} - \frac{i}{\hbar} T_{ni} \int_{t_0}^{t} \underbrace{e^{i\omega_{ni} t' + \varepsilon t'}}\, dt'$$

"T : transition"

ε: regularizes the integral

$e^{t'\varepsilon} \longrightarrow$ integral vanishes as $t_0 \to -\infty$

$\varepsilon > 0$

$t \ll \frac{1}{\varepsilon}$ $\left(\frac{1}{t} \gg \varepsilon \right)$

$\Rightarrow e^{\varepsilon t'} \to 1$ as $t \to \infty$

(take $\varepsilon \to 0$ limit before $t \to \infty$ limit)

Eventually, we need to find a way to calculate T_{ni} ... For now, let's "play" with it and see where it leads us.

Define S-matrix (scattering matrix) through:

$$S_{ni} = \lim_{t\to\infty}\left[\lim_{\varepsilon\to 0} \langle n | \hat{U}_I(t,-\infty) | i\rangle\right]$$

$$= \delta_{ni} - \frac{i}{\hbar} T_{ni} \int_{-\infty}^{\infty} e^{i\omega_{ni}t'} dt'$$

$$= \delta_{ni} - \underbrace{2\pi i\, \delta(E_n - E_i)\, T_{ni}}$$

same math as when we derived Fermi's Golden rule

first part: final state and initial state are the same

this is the second part: Some sort of scattering is happening

If we define the transition rate $w(i\to n) = \frac{d}{dt} |\langle n|\hat{U}_I(t,-\infty)|i\rangle|^2$

then we find:

$$\boxed{w(i\to n) = \frac{2\pi}{\hbar} |T_{ni}|^2 \, \delta(E_n - E_i)}$$

similar to Golden rule, except T (not V)

Independent of time!

Since $w(i\to n)$ is independent of time, we can send t to infinity (nothing will change).

Before working more on T_{ni}, let us imagine that we want to integrate over the final state energy E_n.

$\rightsquigarrow$ need to know the density of states $\rho(E_n)$:

$$\rho(E_n) = \frac{\Delta n}{\Delta E_n}$$

Let $|i\rangle = |\vec{k}\rangle$ and $|n\rangle = |\vec{k}'\rangle$.

In what follows, we assume elastic scattering with $|\vec{k}| = |\vec{k}'| = k$.

$$E_{\vec{n}} = \frac{\hbar^2 \vec{k}'^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |\vec{n}|^2 \Rightarrow \Delta E_{\vec{n}} = \frac{\hbar^2}{m}\left(\frac{2\pi}{L}\right)^2 |\vec{n}|\,\Delta|\vec{n}|$$

particle in a box

$$\vec{n} = n_x\hat{i} + n_y\hat{j} + n_z\hat{k}$$

$$|\vec{n}| = \frac{L}{2\pi}k$$

$$\Delta|\vec{n}| = 4\pi\,|\vec{n}|^2\,\Delta|\vec{n}|\cdot\frac{d\Omega}{4\pi}$$

\# of states within a spherical shell of radius $|\vec{n}|$ and thickness $\Delta|\vec{n}|$

$$\rho(E_{\vec{n}}) = \frac{\Delta|\vec{n}|}{\Delta E_{\vec{n}}} = \frac{4\pi|\vec{n}|^2\,\Delta|\vec{n}|\,\frac{d\Omega}{4\pi}}{\frac{\hbar^2}{m}\left(\frac{2\pi}{L}\right)^2|\vec{n}|\,\Delta|\vec{n}|} = \frac{m}{\hbar^2}\left(\frac{L}{2\pi}\right)^2|\vec{n}|\,d\Omega$$

$$\Rightarrow \rho(E_{\vec{n}}) = \frac{mk}{\hbar^2}\left(\frac{L}{2\pi}\right)^3 d\Omega$$

$|\vec{n}| = \frac{L}{2\pi} k$

$$\Rightarrow w(i \to n) = \frac{m k L^3}{(2\pi)^2 \hbar^3} |T_{ni}|^2 \, d\Omega$$

after integrating over the final states

$$w(i \to n) = \int \frac{2\pi}{\hbar^2} |T_{ni}|^2 \delta(E_n - E_i)\, \rho(E_n)\, dE_n$$

$$= \frac{2\pi}{\hbar^2} |T_{ni}|^2 \rho(E_n)$$

$$d\sigma = \frac{\text{transition rate}}{\text{flux}}$$

$$\text{flux } \vec{j}(\vec{x}, t) = \frac{\hbar}{m} \frac{\vec{k}}{L^3}$$

in general: $\vec{j}(\vec{x}, t) = \frac{\hbar}{m} \mathrm{Im}(\psi^* \nabla \psi)$

$$= \frac{\frac{m k L^3}{(2\pi)^2 \hbar^3} |T_{ni}|^2 \, d\Omega}{\frac{\hbar}{m} \frac{|\vec{k}|}{L^3}}$$

$$\Rightarrow \boxed{\frac{d\sigma}{d\Omega} = \left(\frac{m L^3}{2\pi \hbar^2}\right)^2 |T_{ni}|^2}$$

differential cross section

want to know relationship to $\hat{V}$

So, the differential cross section is determined by the T-matrix!

Even though we don't know yet how to calculate T_{ni}, it is clear now that it will be useful to know T_{ni}.

Recall: All of the discussion so far has been based on first-order time-dependent PT. Eventually, we need to go beyond first-order treatment!

Let's look at calculating T_{ni}:

From the definition:

$$\langle n | \hat{U}_I(t,t_0) | i \rangle = \delta_{ni} - \frac{i}{\hbar} T_{ni} \int_{t_0}^{t} e^{i\omega_{ni}t' + \varepsilon t'} dt'$$

$$\underset{t_0 \to -\infty}{\Rightarrow} \langle n | \hat{U}_I(t,-\infty) | i \rangle = \delta_{ni} + \frac{1}{\hbar} T_{ni} \frac{e^{i\omega_{ni} t + \varepsilon t}}{-\omega_{ni} + i\varepsilon} \quad (*)$$

In interaction picture:

$$\langle n | \hat{U}_I(t,t_0) | i \rangle = \delta_{ni} - \frac{i}{\hbar} \sum_m \underbrace{\langle n | V | m \rangle}_{V_{nm}} \int_{t_0}^{t} e^{i\omega_{nm}t'} \langle m | \hat{U}_I(t',t_0) | i \rangle dt'$$

$$\underset{t_0 \to -\infty}{\Rightarrow} \langle n|\hat{U}_I(t,-\infty)|i\rangle = \delta_{ni} - \frac{i}{\hbar}\sum_m V_{nm}\int_{-\infty}^{t} e^{i\omega_{nm}t'}\langle m|\hat{U}_I(t',-\infty)|i\rangle\, dt' \qquad (**)$$

Plug (*) into integrand of (**):

$$\langle n|\hat{U}_I(t,-\infty)|i\rangle = \delta_{ni}$$

$$\underbrace{}_{\text{from (*): } \delta_{mi} + \frac{1}{\hbar}T_{mi}\left.\frac{e^{i\omega_{mi}t'+\varepsilon t'}}{-\omega_{mi}+i\varepsilon}\right|_{-\infty}^{t}} - \frac{i}{\hbar}\sum_m V_{nm}\int_{-\infty}^{t} e^{i\omega_{nm}t'}\,dt'\;\delta_{mi}$$

$$+\left(\frac{i}{\hbar^2}\right)\sum_m V_{nm}\frac{T_{mi}}{-\omega_{mi}+i\varepsilon}\int_{-\infty}^{t} e^{i\omega_{nm}t'+i\omega_{mi}t'+\varepsilon t'}\,dt'$$

use: $\omega_{nm}+\omega_{mi}=\omega_{ni}$

$$\left.\frac{e^{i\omega_{ni}t'+\varepsilon t'}}{i\omega_{ni}+\varepsilon}\right|_{-\infty}^{t} = \frac{1}{i}\left[\frac{e^{i\omega_{ni}t'+\varepsilon t'}}{\omega_{ni}-i\varepsilon}\right]_{-\infty}^{t}$$

$$= \delta_{ni} - \frac{i}{\hbar}V_{ni}\left.\frac{e^{i\omega_{ni}t'}}{i\omega_{ni}}\right|_{-\infty}^{t}$$

$$+\frac{1}{\hbar^2}\left.\frac{e^{i\omega_{ni}t'+\varepsilon t'}}{\omega_{ni}-i\varepsilon}\right|_{-\infty}^{t}\sum_m V_{nm}\frac{T_{mi}}{-\omega_{mi}+i\varepsilon}$$

Compare l.h.s. and r.h.s. in the $\varepsilon \to 0$ limit:

$$\boxed{T_{ni} = V_{ni} + \underbrace{\lim_{\varepsilon \to 0}}_{} \sum_m V_{nm} \frac{T_{mi}}{E_i - E_m + i\hbar\varepsilon}} \quad (***)$$

this will be dropped: it's implied and executed after the sum over m has been evaluated

Inhomogeneous system of linear equations

→ if V_{nm} are known, we can solve for T_{ni}

We will define another quantity, namely $|\psi^{(+)}\rangle$ in an – at first sight – arbitrary manner:

$$T_{ni} = \langle n | \hat{V} | \psi^{(+)} \rangle = \sum_j \langle n | \hat{V} | j \rangle \langle j | \psi^{(+)} \rangle$$

somehow: when we act w/ $\hat{V}$ onto this state $|\psi^{(+)}\rangle$ and look for the overlap w/ ~~[illegible]~~ the final state, we get T_{ni}

using some basis

Rewrite (∗∗∗) using $|\psi^{(+)}\rangle$:

$$\langle n|\hat{V}|\psi^{(+)}\rangle = \langle n|\hat{V}|i\rangle + \langle n|\hat{V}\sum_m \frac{|m\rangle\langle m|\hat{V}|\psi^{(+)}\rangle}{E_i - E_m + i\hbar\varepsilon}$$

Since this holds for any $|n\rangle$, we can write:

$$|\psi^{(+)}\rangle = |i\rangle + \sum_m \frac{\langle m|\hat{V}|\psi^{(+)}\rangle}{E_i - E_m + i\hbar\varepsilon}|m\rangle$$

$$= |i\rangle + \sum_m \frac{\langle m|\hat{V}|\psi^{(+)}\rangle}{E_i - \hat{H}_0 + i\hbar\varepsilon}|m\rangle$$

$$= |i\rangle + \underbrace{\sum_m |m\rangle\langle m|}_{=\mathbb{1}}\frac{\hat{V}|\psi^{(+)}\rangle}{E_i - \hat{H}_0 + i\hbar\varepsilon}$$

$$\Rightarrow \boxed{|\psi^{(+)}\rangle = |i\rangle + \frac{1}{E_i - \hat{H}_0 + i\hbar\varepsilon}\hat{V}|\psi^{(+)}\rangle}$$

Lippmann-Schwinger equation

We don't really have a feeling for the physical meaning of $|\psi^{(+)}\rangle$ yet... To see what $|\psi^{(+)}\rangle$ represents, we want to look at $\langle\vec{x}|\psi^{(+)}\rangle$ in the limit that $|\vec{x}|$ is large. Let's postpone this for a little while.

We had defined $|\psi^{(+)}\rangle$ through $T_{ni} = \langle n|\hat{V}|\psi^{(+)}\rangle$.

We had defined T_{ni} as complex numbers through

$$\langle n|\hat{U}_I(t,t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar} T_{ni} \int_{t_0}^{t} e^{i\omega_{ni}t' + \varepsilon t'} dt'$$

We now define an operator $\hat{T}$ through

$$\hat{T}|i\rangle = \hat{V}|\psi^{(+)}\rangle$$

$$\Rightarrow \langle n|\hat{T}|i\rangle = \underbrace{\langle n|\hat{V}|\psi^{(+)}\rangle}_{T_{ni}}$$

so: this all checks out in terms of consistency...

go back to $|\psi^{(+)}\rangle = |i\rangle + \frac{1}{E_i - \hat{H}_0 + i\hbar\varepsilon} \hat{V}|\psi^{(+)}\rangle$

and act on the equation with $\hat{V}$:

$$\underbrace{\hat{V}|\psi^{(+)}\rangle}_{\hat{T}|i\rangle} = \hat{V}|i\rangle + \hat{V}\frac{1}{E_i - \hat{H}_0 + i\hbar\varepsilon}\underbrace{\hat{V}|\psi^{(+)}\rangle}_{\hat{T}|i\rangle}$$

$$\Rightarrow \boxed{\hat{T} = \hat{V} + \hat{V}\frac{1}{E_i - \hat{H}_0 + i\hbar\varepsilon}\hat{T}}$$

operator equation

Let's iterate:

$$\hat{T} \approx \hat{V} + \hat{V} \frac{1}{E_i - \hat{H}_0 + i\hbar\varepsilon} \hat{V} + \hat{V} \frac{1}{\cdots} \hat{V} \frac{1}{\cdots} \hat{V} + \ldots$$

assuming
$\hat{V}$ is weak
(need to determine
what it means when
we say that an operator
is weak ...)

This operator equation forms the basis for the Born-approximation (see Sec. 6.3)

Let's again go back and look at how we defined T_{ni}:

$$\langle n | \hat{U}_I(t, t_0) | i \rangle = \delta_{ni} - \frac{i}{\hbar} T_{ni} \int_{t_0}^{t} e^{i\omega_{ni} t' + \varepsilon t'} dt'$$

we then sent $t_0 \to -\infty$, i.e., we looked at going from the past to the future ($\varepsilon > 0$ but small)

Now:

$$\langle n | \hat{U}_I(t, t_0) | i \rangle = \delta_{ni} + \frac{i}{\hbar} T_{ni} \int_{t}^{t_0} e^{i\omega_{ni} t' - \varepsilon t'} dt'$$

switching integration limits

use opposite sign

we use the opposite sign!

we can now send $t_0 \to \infty$, i.e., we are looking at going from the future to the past (again, ε small and positive).

In this case, we define the operator $\hat{T}$ through

$$\hat{T}|i\rangle = \hat{V}|\psi^{(-)}\rangle$$

$|\psi^{(+)}\rangle$ and $|\psi^{(-)}\rangle$ are two different scattering kets!

They play a key role in scattering theory.

We will see: $\langle\vec{x}|\psi^{(+)}\rangle \mathrel{\hat{=}}$ outgoing

$\langle\vec{x}|\psi^{(-)}\rangle \mathrel{\hat{=}}$ incoming

6.2 Scattering Amplitude

We will redefine ε: $\hbar\varepsilon \rightarrow \varepsilon$ (simplifies notation)

Then:

$$|\psi^{(\pm)}\rangle = |i\rangle + \frac{1}{E - \hat{H}_0 \pm i\varepsilon} \hat{V} |\psi^{(\pm)}\rangle$$

$$\Rightarrow \langle \vec{x} | \psi^{(\pm)} \rangle = \langle \vec{x} | i \rangle + \int \langle \vec{x} | \frac{1}{E - \hat{H}_0 \pm i\varepsilon} | \vec{x}' \rangle \langle \vec{x}' | \hat{V} | \psi^{(\pm)} \rangle \, d^3\vec{x}'$$

come in from left with $\langle \vec{x}|$ and insert complete set of position-basis states

$$\int |\vec{x}'\rangle\langle\vec{x}'| \, d^3\vec{x}' = \hat{\mathbb{1}}$$

note: the subscript of the energy got dropped. E is still eigenenergy of ket $|i\rangle$

The ket $|\psi^{(\pm)}\rangle$ appears in integrand $\rightsquigarrow$ so, this is an integral equation for $|\psi^{(\pm)}\rangle$

We also have $\langle \vec{x} | \frac{1}{E - \hat{H}_0 \pm i\varepsilon} | \vec{x}' \rangle$ in the integrand. Let's give this a name and then let's find a "usable" expression.

$$\boxed{G_\pm(\vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \langle \vec{x} | \frac{1}{E - \hat{H}_0 \pm i\varepsilon} | \vec{x}' \rangle}$$

Green's function (we'll see later how it relates to Helmholtz equation)

Let's insert complete sets: $\sum_{\vec{k}} |\vec{k}'\rangle\langle\vec{k}'| = \hat{1}$

$$\sum_{\vec{k}'} |\vec{k}''\rangle\langle\vec{k}''| = \hat{1}$$

$$G_\pm(\vec{x},\vec{x}') = \frac{\hbar^2}{2m}\sum_{\vec{k}'}\sum_{\vec{k}''} \underbrace{\langle\vec{x}|\vec{k}'\rangle}_{\frac{e^{i\vec{k}'\cdot\vec{x}}}{L^{3/2}}} \underbrace{\langle\vec{k}'|\frac{1}{E-\hat{H}_0 \pm i\varepsilon}|\vec{k}''\rangle} \underbrace{\langle\vec{k}''|\vec{x}'\rangle}_{\frac{e^{-i\vec{k}''\cdot\vec{x}'}}{L^{3/2}}}$$

$$\langle\vec{k}'|\frac{1}{E-\frac{\hbar^2\vec{k}''^2}{2m}\pm i\varepsilon}|\vec{k}''\rangle$$

$$= \delta_{\vec{k}'\vec{k}''}\frac{1}{E-\frac{\hbar^2\vec{k}'^2}{2m}\pm i\varepsilon}$$

$$= \frac{1}{L^3}\sum_{\vec{k}'}\frac{e^{i\vec{k}'\cdot(\vec{x}-\vec{x}')}}{k^2-\vec{k}'^2\pm i\varepsilon}$$

we redefined ε: $\varepsilon \to \frac{2m\varepsilon}{\hbar^2}$

Convert $\sum_{\vec{k}'}$ to integral: $k_x = \frac{2\pi}{L}n_x$, $k_y = \ldots$, $k_z = \ldots$

$$\Rightarrow \sum_{\vec{k}'} \longrightarrow \left(\frac{L}{2\pi}\right)^3 \int \ldots d^3\vec{k}'$$

$$\Rightarrow G_\pm(\vec{x}, \vec{x}\,') = \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{k}'\cdot(\vec{x}-\vec{x}\,')}}{k^2 - k'^2 \pm i\varepsilon} \, d^3\vec{k}'$$

$$= \frac{1}{(2\pi)^3} \iiint \frac{e^{ik'|\vec{x}-\vec{x}\,'|\cos\theta}}{k^2 - k'^2 \pm i\varepsilon} \, k'^2 dk' \, d\hat{\vec{k}}'$$

θ: angle between $\vec{k}'$ and $|\vec{x} - \vec{x}\,'|$

$$\cos\theta = \mu$$

$$\underbrace{d\cos\theta}_{-\sin\theta \, d\theta} = d\mu$$

$$= \frac{2\pi}{(2\pi)^3} \int_0^\infty (-1) \underbrace{\int_{+1}^{-1} \frac{e^{ik'|\vec{x}-\vec{x}\,'|\mu}}{k^2 - k'^2 \pm i\varepsilon} \, d\mu}_{\frac{-1}{ik'|\vec{x}-\vec{x}\,'|} \left. \frac{e^{ik'|\vec{x}-\vec{x}\,'|\mu}}{k^2 - k'^2 \pm i\varepsilon} \right|_{+1}^{-1}} \, k'^2 dk'$$

$$= \frac{-1}{ik'|\vec{x}-\vec{x}\,'|} \frac{e^{-ik'|\vec{x}-\vec{x}\,'|} - e^{ik'|\vec{x}-\vec{x}\,'|}}{k^2 - k'^2 \pm i\varepsilon}$$

$$= \frac{-1}{4\pi^2 i} \int_0^\infty \frac{1}{|\vec{x}-\vec{x}\,'|} \frac{e^{-ik'|\vec{x}-\vec{x}\,'|} - e^{ik'|\vec{x}-\vec{x}\,'|}}{k^2 - k'^2 \pm i\varepsilon} \, k' dk'$$

$$= \Bigg[\frac{1}{4\pi^2 i}\int_0^\infty \frac{e^{ik'|\vec{x}-\vec{x}'|}}{k^2-k'^2 \pm i\varepsilon}\, k'\,dk'$$

$$- \underbrace{\frac{1}{4\pi^2 i}\int_0^\infty \frac{e^{-ik'|\vec{x}-\vec{x}'|}}{k^2-k'^2 \pm i\varepsilon}\, k'\,dk'}\Bigg]\frac{1}{|\vec{x}-\vec{x}'|}$$

let $k' = -k''$

$$\int_0^{-\infty} \frac{e^{ik''|\vec{x}-\vec{x}'|}}{k^2-k''^2 \pm i\varepsilon}\, k''\,dk''$$

$$= -\int_{-\infty}^{0} \frac{e^{ik'|\vec{x}-\vec{x}'|}}{k^2-k'^2 \pm i\varepsilon}\, k'\,dk'$$

$k''=k'$ (renaming again)

$$= \frac{1}{4\pi^2 i\,|\vec{x}-\vec{x}'|}\int_{-\infty}^{\infty} \frac{e^{ik'|\vec{x}-\vec{x}'|}}{k^2-k'^2 \pm i\varepsilon}\, k'\,dk'$$

$-(k'^2 - k^2 \mp \varepsilon)^{-1}$ has poles when

$k'^2 = k^2 \pm i\varepsilon$

Write: $-\left[k' - (k_r \pm i\frac{k_i}{2k_r})\right]\left[k' + (k_r \pm i\frac{k_i}{2k_r})\right]$

$$= -\left[k'^2 - (k_r \pm i\frac{k_i}{2k_r})^2\right]$$

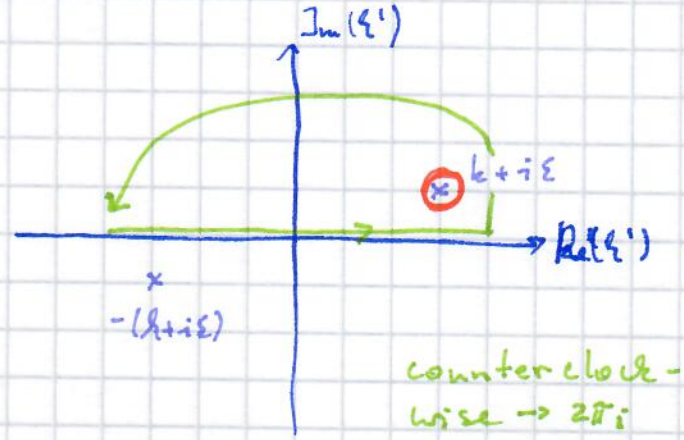
$$= -\left[k'^2 - k_r^2 \mp i k_i + O\left((k_i/2k_r)^2\right)\right]$$

So: we have an integral like

$$J = -\int_{-\infty}^{\infty} \frac{e^{ik'|\vec{x}-\vec{x}'|}\, k'}{[k' - (k \pm i\varepsilon)][k' + (k \pm i\varepsilon)]}\, dk'$$

here, I redefined what ε is

For $+i\varepsilon$ (ε positive):



Close contour in the upper half plane:

the point encircled in orange is enclosed by the contour

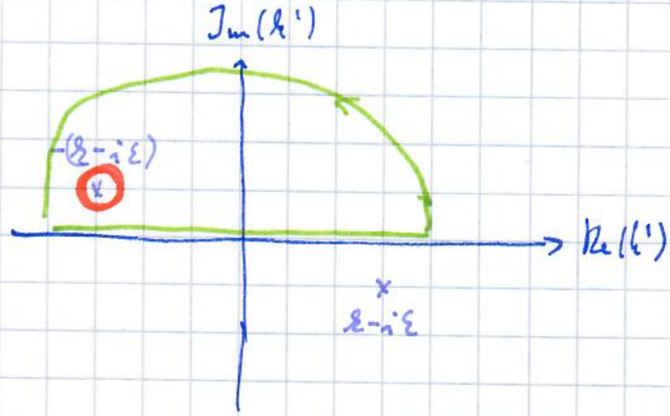
for $k' = k + i\varepsilon$, we have:

$$e^{i(k+i\varepsilon)|\vec{x}-\vec{x}'|} = e^{ik|\vec{x}-\vec{x}'|}\underbrace{e^{-\varepsilon|\vec{x}-\vec{x}'|}}_{\substack{\text{falls off} \\ (\varepsilon \text{ positive})}}$$

By residue theorem

$$J = -(2\pi i)\, \frac{e^{ik|\vec{x}-\vec{x}'|}}{2k}\, k$$

For $-i\varepsilon$ (ε positive):



counterclockwise
$\rightarrow 2\pi i$

Close contour in upper half plane

the point encircled in orange is enclosed by the contour

for $k' = -(k - i\varepsilon)$, we have

$$e^{-i(k-i\varepsilon)|\vec{x}-\vec{x}'|} = e^{-ik|\vec{x}-\vec{x}'|} \underbrace{e^{-\varepsilon|\vec{x}-\vec{x}'|}}_{\text{falls off } (\varepsilon \text{ positive})}$$

By residue theorem:

$$J = -(2\pi i)\, \frac{e^{-ik|\vec{x}-\vec{x}'|}(-k)}{2(-k)}$$

Altogether: $J = - \pi i \; e^{\pm ik|\vec{x}-\vec{x}'|}$

$$\Rightarrow \boxed{G_{\pm}(\vec{x},\vec{x}') = - \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|}}$$

$$G_+(\vec{x},\vec{x}') = -\frac{1}{4\pi|\vec{x}-\vec{x}'|}\, e^{ik|\vec{x}-\vec{x}'|} \qquad \text{"outgoing"}$$

$$G_-(\vec{x},\vec{x}') = -\frac{1}{4\pi|\vec{x}-\vec{x}'|}\, e^{-ik|\vec{x}-\vec{x}'|} \qquad \text{"incoming"}$$

$G_\pm(\vec{x},\vec{x}')$ solves the Helmholtz equation:

$$\left(\nabla^2 + k^2\right) G_\pm(\vec{x},\vec{x}') = \delta^{(3)}(\vec{x}-\vec{x}')$$

So: for $\vec{x} \neq \vec{x}'$, $G_\pm(\vec{x},\vec{x}')$ solves the eigenvalue equation

$$\hat{H}_0\, G_\pm(\vec{x},\vec{x}') = E\, G_\pm(\vec{x},\vec{x}'). \quad (\vec{x}\neq\vec{x}')$$

This was a lot of work... Recall: we had the following expression:

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \langle\vec{x}|i\rangle + \frac{2m}{\hbar^2}\int G_\pm(\vec{x},\vec{x}')\langle\vec{x}'|\hat{V}|\psi^{(\pm)}\rangle d^3\vec{x}'$$

Plug in for $G_\pm(\vec{x},\vec{x}')$:

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \underbrace{\langle\vec{x}|i\rangle}_{\text{incident}} \underbrace{- \frac{2m}{\hbar^2}\int \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|}\langle\vec{x}'|\hat{V}|\psi^{(\pm)}\rangle d^3\vec{x}'}_{\text{"scattered"}}$$

$\frac{e^{ikr}}{r}$ outgoing (forward in time) | $\frac{e^{-ikr}}{r}$ incoming (backward in time)

We want to understand the "scattered" part better.

Restrict ourselves to so-called local potentials:

$$\langle \vec{x}' | \hat{V} | \vec{x}'' \rangle = V(\vec{x}')\, \delta^{(3)}(\vec{x}' - \vec{x}'')$$

For local potentials:

$$\langle \vec{x}' | \hat{V} | \psi^{(\pm)} \rangle = \int \underbrace{\langle \vec{x}' | \hat{V} | \vec{x}'' \rangle}_{V(\vec{x}')\,\delta^{(3)}(\vec{x}'-\vec{x}'')} \langle \vec{x}'' | \psi^{(\pm)} \rangle \, d^3\vec{x}''$$

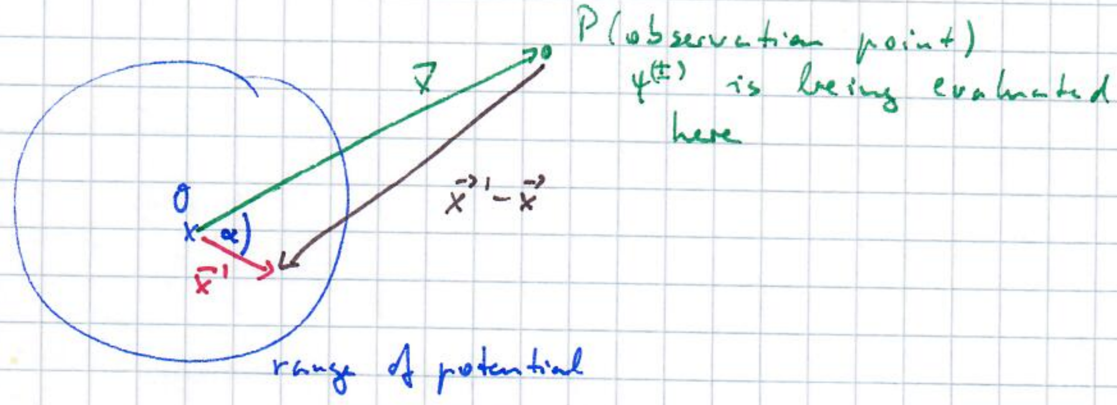
inserting complete set / closure

$$= V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle$$

using that $\hat{V}$ is local by assumption

It follows:

$$\langle \vec{x} | \psi^{(\pm)} \rangle = \langle \vec{x} | i \rangle - \frac{2m}{\hbar^2} \int \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi |\vec{x} - \vec{x}'|} V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle$$



Since the observation is always made at a detector that is far away from the scatterer, we have:

$$|\vec{x}| = r \gg |\vec{x}'| = r'$$

$$\Rightarrow |\vec{x} - \vec{x}'| = \sqrt{r^2 - 2rr'\cos\alpha + r'^2}$$

α is the angle between $\vec{x}$ and $\vec{x}'$

$$= r\left(1 - 2\frac{r'}{r}\cos\alpha + \left(\frac{r'}{r}\right)^2\right)^{1/2}$$

Taylor exp.

$$\approx r\left(1 - \vec{x}\cdot\vec{x}'\right)$$

defining $\hat{r} = \frac{\vec{x}}{r}$

$$= r - \hat{r}\cdot\vec{x}'$$

$$\Rightarrow \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \approx \frac{1}{r}\, e^{\pm ikr}\, e^{\mp i\vec{k}'\cdot\vec{x}'}$$

using $\frac{1}{|\vec{x}-\vec{x}'|} \approx \frac{1}{r}$

and defining $\vec{k}' = k\,\hat{r}$

Let's use $|i\rangle = |\vec{k}\rangle$, i.e., initial state is eigenket of Hamiltonian $\hat{H}_0$.

$$\Rightarrow \langle \vec{x} | \psi^{(\pm)} \rangle \xrightarrow[\text{large } r]{} \langle \vec{x} | \vec{k} \rangle - \frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle \, d^3\vec{x}'$$

$$= \langle \vec{x} | \vec{k} \rangle - \frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{r} \int \langle \vec{k}' | \vec{x}' \rangle V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle \, d^3\vec{x}'$$

$$= \frac{1}{L^{3/2}} \left[e^{i\vec{k}\cdot\vec{x}} + \frac{e^{ikr}}{r} f(\vec{k}', \vec{k}) \right]$$

where

$$\boxed{\begin{aligned} f(\vec{k}', \vec{k}) &= -\frac{mL^3}{2\pi\hbar^2} \int \frac{e^{-i\vec{k}'\cdot\vec{x}'}}{L^{3/2}} V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle \, d^3\vec{x}' \\ &= -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | \hat{V} | \psi^{(\pm)} \rangle \end{aligned}}$$

Scattering amplitude

Differential scattering cross section $\frac{d\sigma}{d\Omega}$:

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}', \vec{k})|^2$$

this can be seen by looking at our earlier expression:

$$\frac{d\sigma}{d\Omega} = \left(\frac{mL^3}{2\pi\hbar^2} \right)^2 |\langle n | V | \psi^{(\pm)} \rangle|^2$$

Optical theorem (w/o proof):

$$\mathrm{Im}\, \underbrace{f(\theta=0)}_{f(\vec{k},\vec{k})} = \frac{k}{4\pi}\, \sigma_{tot}$$

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega}\, d\Omega$$

6.3 The Born Approximation

We want to calculate $f(\vec{k}', \vec{k})$ to get

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}', \vec{k})|^2$$

Recall $f(\vec{k}', \vec{k}) = -\frac{mL^3}{2\pi\hbar^2} \underbrace{\langle \vec{k}' | \hat{V} | \psi^{(+)} \rangle}_{\langle \vec{k}' | \hat{T} | \vec{k} \rangle}$

This is still challanging $\rightsquigarrow$ we don't have explicit expression for $\hat{T}$ or $\psi^{(+)}(\vec{x}')$.

Let's go back to operator equation (6.1.31) (with $\hbar\varepsilon$ replaced by ε)

$$\hat{T} = \hat{V} + \hat{V} \frac{1}{E_i - \hat{H}_0 + i\varepsilon} \hat{T}$$

Let's iterate this once:

$$\hat{T} = \hat{V} + \hat{V} \frac{1}{E_i - \hat{H}_0 + i\varepsilon} \left[\hat{V} + \hat{V} \frac{1}{E_i - \hat{H}_0 + i\varepsilon} \hat{T} \right]$$

$$= \hat{V} + \hat{V} \frac{1}{E_i - \hat{H}_0 + i\varepsilon} \hat{V} + \hat{V} \frac{1}{E_i - \hat{H}_0 + i\varepsilon} \hat{V} \frac{1}{E_i - \hat{H}_0 + i\varepsilon} \hat{T}$$

$$= (\text{term w/ } 1\,\hat{V}) + (\text{term w/ } \hat{V} \ldots \hat{V}) + (\text{term w/ } \hat{V} \ldots \hat{V} \ldots \hat{V}) + \ldots$$

if we iterate again

So: we have an expansion in terms of $\hat{V}$.

Let's cut the series off after the first term: $\hat{T} \approx \hat{V}$

Then:

$$f^{(1)}(\vec{k}', \vec{k}) = -\frac{m L^3}{2\pi\hbar^2} \langle \vec{k}' | \hat{V} | \vec{k} \rangle$$

Scattering amplitude in first-order Born-approximation

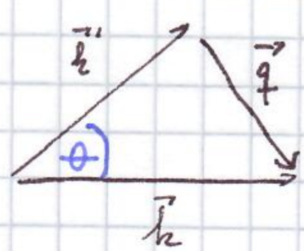
$$= -\frac{m}{2\pi\hbar^2} \int e^{i(\vec{k}-\vec{k}')\cdot\vec{x}'} V(\vec{x}')\, d^3\vec{x}'$$

$$= -\frac{m}{2\pi\hbar^2} \underbrace{\int e^{i\vec{q}\cdot\vec{x}'} V(\vec{x}')\, d^3\vec{x}'}_{\text{3D Fourier transformation of the potential w/ respect to } \vec{q}}$$

$\vec{q} = \vec{k} - \vec{k}'$

If $\underbrace{V(\vec{x}') = V(|\vec{x}'|)}_{\text{spherically symmetric interaction potential}}$, then: $q = |\vec{k} - \vec{k}'|$

$\hookrightarrow f^{(1)}(\vec{k}', \vec{k})$ only depends on q.



$|\vec{k}'| = k$ by energy conservation

$q = 2k \sin\frac{\theta}{2}$

To evaluate $f^{(1)}(\vec{k}', \vec{k})$, we write $\vec{q} \cdot \vec{x}' = q\,|\vec{x}'| \cos\alpha$.

The angular integration can be performed analytically (see HW) and we arrive at

$$f^{(1)}(\vec{k}', \vec{k}) = -\frac{2m}{\hbar^2}\frac{1}{q}\underbrace{\int_0^\infty r\,V(r)\sin(qr)\,dr}$$

to evaluate this, we need to know the form of the potential

Let's take another look at general form of $f^{(1)}(\vec{k}'; \vec{k})$:

$$f^{(1)}(\vec{k}', \vec{k}) = -\frac{m}{2\pi\hbar^2}\int \underbrace{e^{-i\vec{k}'\cdot\vec{x}'}}_{\text{"outgoing": plane wave}} V(\vec{x}')\,\underbrace{e^{i\vec{k}\cdot\vec{x}'}}_{\text{"incoming": plane wave}}\,d^3\vec{x}'$$

⟶ this is like in first-order perturbation theory: for first order, the plane wave that's coming in is not changed, except that the direction of the wave vector has changed

Is the Born-approximation (at first-order) any good?

To answer this question, let us connect the BA with the full expression:

$$\langle \vec{x} | \psi^{(+)} \rangle = \langle \vec{x} | \vec{k} \rangle \underbrace{- \frac{2m}{\hbar^2} \int \frac{e^{ik|\vec{x}-\vec{x}'|}}{4\pi |\vec{x}-\vec{x}'|} V(\vec{x}') \langle \vec{x}' | \psi^{(+)} \rangle d^3x'}$$

this term must be much smaller than the first term (want to look at absolute value and specific $\vec{x}$ value)

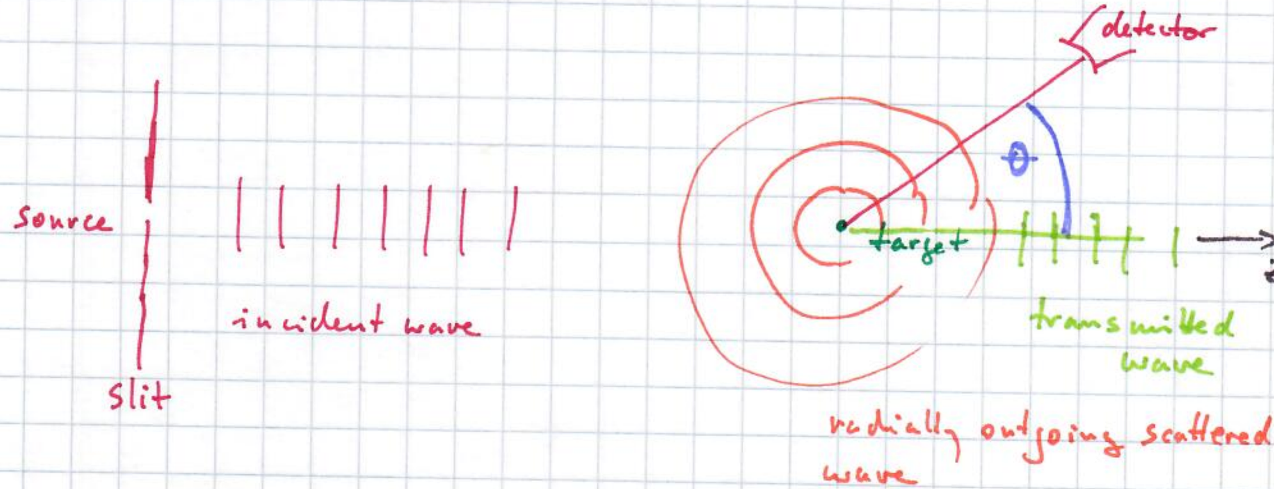
Estimating that the potential has a depth V_0 and a range a, the validity criterium becomes

$$\frac{m |V_0| a^2}{\hbar^2} \ll 1 \quad \text{(assumes } ka \ll 1\text{)}$$

→ Usually, this means that the potential does not support a bound state

→ So, in some sense, the Born-approximation requires a "small parameter" (but it's not as simple as one small number)

6.4 Phase shifts and partial waves

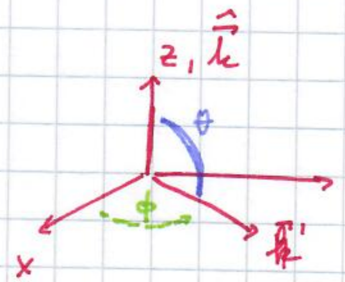


incoming particle $\vec{k}$

scattered particle $\vec{k}'$

detection at angles θ and ϕ

(θ and ϕ locate detector relative to beam direction)



ϕ angle in xy plane

Dimension of incoming wave packet is much larger than the typical range of the interaction potential (i.e., the size of the scatterer)

We are interested in elastic scattering: $|\vec{k}| = |\vec{k}'|$

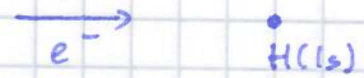
initial energy is equal to final energy

but $\vec{k}$ and $\vec{k}'$ can point in different directions

Another small aside: We assume that the collision energy is relatively small

$\rightarrow$ no relativistic quantum mechanics needed

As an example, let's look at $e^- + H(1s)$ scattering:



Condition for elastic scattering? What energy of e^- guarantees elastic scattering?

$e^- + H(1s) \rightarrow e^- + H(1s)$

energy of e^- must be less than 10.2 eV!

Why? $\underbrace{13.6\,eV}_{\text{gr. st.}} - \underbrace{3.4\,eV}_{\text{first exc. st.}}$

If energy of $e^- > 10.2\,eV$, then other fragmentation channels become available.

inelastic scattering $\left\{ \begin{array}{l} e^- + H(1s) \rightarrow e^- + \underbrace{H^*}_{\begin{array}{c} H(2s) \\ H(2p) \\ \vdots \end{array}} \end{array} \right.$

multi-channel scattering $\Big\{$ for $> 13.6\,eV$: fragmentation channels become open

$e^- + H(1s) \rightarrow e^- + e^- + p$

Formal description of free incoming wave packet:

$$\Psi(\vec{x},t) = \frac{1}{L^{3/2}} \int e^{i(\vec{k}''\cdot\vec{x} - E_{k''}t/\hbar)} A(\vec{k}'')\, d^3\vec{k}''$$

But we said that we want a broad wave packet!

This means that $A(\vec{k}'')$ must be sharply peaked around $\vec{k}$:

"initial $\vec{k}$" $\qquad A(\vec{k}'') = \delta(\vec{k}'' - \vec{k})$

$$\Rightarrow \Psi(\vec{x},t) = \frac{1}{L^{3/2}}\, e^{i(\vec{k}\cdot\vec{x} - \underbrace{E_k t/\hbar}_{})}$$

but: energy is conserved during the scattering process: no need to keep the time dependence explicitly

Infinitely sharp momentum $\longleftrightarrow$ fully delocalized particle

According to our schematic:

$$\psi(\vec{x}) \xrightarrow[|\vec{x}| \to \infty]{} \psi_{inc}(\vec{x}) + \psi_{sc}(\vec{x})$$

We assume that the detector is placed "outside" the incident beam $\rightsquigarrow$ only scattered particles are recorded.

We write the $|\vec{x}| \to \infty$ wave function as:

$$\psi^{(+)}(\vec{x}) \to \frac{1}{L^{3/2}} \left[e^{i\vec{k}\cdot\vec{x}} + f(\vec{k}', \vec{k}) \frac{e^{ik|\vec{x}|}}{|\vec{x}|} \right]$$

This can be viewed as an asymptotic boundary condition. We don't know what happens during the scattering process (black box) but we do know what form of the wave fct. we expect. We simply call the prefactor of the spherically outgoing wave $f(\vec{k}', \vec{k})$.

Let's recall how we treated scattering in classical mechanics.

$$\frac{d\sigma}{d\Omega} = \frac{\text{outgoing flux of particles passing through area } |\vec{x}|^2\, d\Omega \text{ per unit solid angle}}{\text{incident flux}}$$

$d\Omega = \sin\theta \, d\theta \, d\phi$

$d\Omega = d\hat{k}'$

Let's work this out:

$$\vec{j} = \frac{\hbar}{2mi}\left(\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right)$$

$$\psi_{inc} = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{x}}$$

$$\Rightarrow \quad \vec{j}_{inc} = \frac{1}{L^3} \underbrace{\frac{\hbar}{m} k}_{v} \hat{k}$$

If we let $\vec{k}$ lie along $\hat{z}$, then the flux along z is $\vec{j}_{inc} \cdot \hat{z} = \frac{1}{L^3}\frac{\hbar k}{m} = j_{inc}$

Next, let's look at the scattered part:

$$\psi_{sc}(\vec{x}) = \frac{1}{L^{3/2}} \frac{e^{ik|\vec{x}|}}{|\vec{x}|} f(\vec{k}', \vec{k})$$

$$\Rightarrow \underbrace{\vec{j}_{sc} \cdot \hat{\vec{x}}'}_{\text{radial current}} = \frac{\hbar}{2mi}\left(\psi_{sc}^* \frac{\partial}{\partial|\vec{x}|}\psi_{sc} - \psi_{sc}\frac{\partial}{\partial|\vec{x}|}\psi_{sc}^*\right)$$

only the radial derivative contributes

$$= \underbrace{\frac{1}{L^3}\frac{\hbar k}{m}}_{j_{inc}} \frac{1}{|\vec{x}|^2} \left|f(\vec{k}', \vec{k})\right|^2$$

Putting it together:

$$\boxed{\frac{d\sigma}{d\Omega} = \left|f(\vec{k}', \vec{k})\right|^2}$$

this is, of course, consistent w/ what we did in Sec. 6.2

For what follows, we will assume that the potential is spherically symmetric:

$$V(\vec{x}) = V(|\vec{x}|)$$

We will let $\vec{k}$ lie along $\hat{z}$.

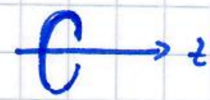
In general, we need ~~θ~~ and ϕ to describe $\vec{k}'$.

However, for a spherically symmetric potential, we have an azimuthal symmetry, i.e., $f(\vec{k}', \vec{k})$ will simplify:

$$f(\vec{k}', \vec{k}) \rightsquigarrow f(k, \theta)$$

along $\hat{z}$

no ϕ dependence



Goal: Find an expression for $f(k, \theta)$ such that we can calculate $d\sigma/d\Omega$ easily. We already looked at one approach. In what follows, we learn about an alternative formulation.

Idea: Write $\psi^{(+)}(\vec{x})$ in two different ways. Comparison of the two ways of writing things gives $f(k, \theta)$.

expression for it can be "read off"

Approach (i) : $\psi^{(+)}(\vec{x}) \xrightarrow[|\vec{x}|\to\infty]{} \frac{1}{L^{3/2}}\left[e^{ikz} + f(k,\theta)\, e^{ikr}/r\right]$

(recall: $|\vec{x}| = r$)

rewrite these pieces

$$e^{ikz} = \sum_{\ell}(2\ell+1)\, i^{\ell}\, j_{\ell}(kr)\, P_{\ell}(\cos\theta)$$

Approach (ii) : Forget about $f(k,\theta)$ and expand $\psi^{(+)}(\vec{x})$ "as usual"

Let's start with approach (ii):

$$\psi^{(+)}(\vec{x}) = \sum_{\ell=0}^{\infty} \underbrace{R_{\ell}(k,r)}_{\text{unknown}}\, P_{\ell}(\cos\theta)$$

(no n label since we have no quantization condition)

$$P_{\ell}(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_{\ell 0}(\theta,\phi)$$

Legendre polynomial: they form a complete set in $-1 \le \cos\theta \le 1$ (no ϕ dependence)

To determine unknown $R_\ell(k,r)$, plug $\psi^{(+)}(\vec{x})$ into S.E.:

$$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(r)\right)\psi^{(+)}(\vec{x}) = E\psi^{(+)}(\vec{x})$$

Simplify, taking advantage of the fact that $V(r)$ is spherically symmetric:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r)\right] R_\ell(k,r) = E R_\ell(k,r)$$

Now let $\frac{u_\ell(k,r)}{r} = R_\ell(k,r)$:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r)\right) u_\ell(k,r) = E u_\ell(k,r)$$

So far, we have not placed any restrictions on r. We are, however, interested in determining $R_\ell(k,r)$ in the large r limit: $\underbrace{V(r) \to 0 \text{ as } r \to \infty}$

Requires: $V(r)$ falls off faster than r^{-2}

We want $\frac{\hbar^2 \ell(\ell+1)}{2mr^2}$ to dominate over $V(r)$.

$$R_\ell(k,r) \xrightarrow{r\to\infty} B_\ell(k)\, \underbrace{j_\ell(kr)}_{\text{spherical Bessel fct.}} + C_\ell(k)\, \underbrace{n_\ell(kr)}_{\text{Neumann fct.}}$$

two unknown that depend on the scattering energy

$j_\ell(kr)$ is regular at the origin:

$$j_\ell(kr) \longrightarrow \frac{(kr)^\ell}{(2\ell+1)!!}$$

$n_\ell(kr)$ is irregular at the origin:

$$n_\ell(kr) \longrightarrow -\frac{(2\ell-1)!!}{(kr)^{\ell+1}}$$

$$(2\ell-1)!! = 1\cdot 3\cdot 5 \cdot \ldots \cdot (2\ell-1)$$

$$(2\ell-1)!! = 1 \quad \text{for } \ell = 0$$

Also:

$$j_\ell(kr) \xrightarrow[kr \gg 1]{} \frac{\sin\left(kr - \frac{\ell\pi}{2}\right)}{kr}$$

$$n_\ell(kr) \xrightarrow[kr \gg 1]{} -\frac{\cos\left(kr - \frac{\ell\pi}{2}\right)}{kr}$$

$$R_\ell(k,r) \xrightarrow[r\to\infty]{} B_\ell(k)\left[j_\ell(kr) - \underbrace{\left(\frac{-C_\ell(k)}{B_\ell(k)}\right)}_{\tan(\delta_\ell(k))} n_\ell(kr)\right]$$

"replace the name"

$$= B_\ell(k)\left[j_\ell(kr) - \tan(\delta_\ell(k))\, n_\ell(kr)\right]$$

$$\xrightarrow[kr\gg 1]{} \frac{A_\ell(k)}{kr} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)$$

(using trig identities)

$$A_\ell(k) = \sqrt{B_\ell^2(k) + C_\ell^2(k)}$$

This is almost the end of approach (ii). We simply wrote the asymptotic free particle solution in terms of the phase shifts $\delta_\ell(k)$. $\tan(\delta_\ell(k))$ tells us the relative importance of the regular and irregular solution. If we don't have a potential, then we will only have the regular solution, i.e., all $\delta_\ell(k)$ will be zero. When we have a potential, the $\delta_\ell(k)$ will, in general, not be zero. The values of $\delta_\ell(k)$ can be viewed as a signature of $V(r)$.

For later reference, it will be good to rewrite the $\sin()$ in terms of exponentials:

$$\sin x = \frac{1}{2i}\left(e^{ix} - e^{-ix}\right)$$

$$R_\ell(kr) \xrightarrow[kr \gg 1]{} A_\ell(k)\left[\frac{e^{ikr}}{r}\,\frac{e^{-i\ell\pi/2}\,e^{i\delta_\ell(k)}}{2ik}\right.$$

$$\left. - \frac{e^{-ikr}}{r}\,\frac{e^{i\ell\pi/2}\,e^{-i\delta_\ell(k)}}{2ik}\right]$$

This will come in handy when we compare with the result of approach (i).

Before going to approach (i), it should be noted that we can find the $\delta_\ell(k)$ by solving the radial SE for a specific $V(r)$ for each ℓ and by then looking at the solution in the limit that $kr \gg 1$.

Next, we want to rewrite $\psi^{+}(\vec{x})$, written in terms of $f(k,\theta)$ (approach (i)):

Recall: $\psi^{(+)}(\vec{x}) \propto e^{ikz} + f(k,\theta)\,\frac{e^{ikr}}{r}$

$$\Big\downarrow$$

$$e^{ikz} = \sum_\ell (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos\theta)$$

But: $j_\ell(kr) \xrightarrow[kr\gg 1]{} \frac{\sin(kr - \ell\pi/2)}{kr}$

$$= \frac{1}{2ikr}\left[e^{i(kr-\frac{\ell\pi}{2})} - e^{-i(kr-\frac{\ell\pi}{2})}\right]$$

So: $\psi^{(+)}(\vec{x}) \propto \frac{e^{ikr}}{r}\left[f(k,\theta) + \sum_\ell \frac{(2\ell+1)\, i^\ell\, e^{-i\ell\pi/2}\, P_\ell(\cos\theta)}{2ik}\right]$

$$+ \frac{e^{-ikr}}{r}\left[\sum_\ell \frac{-(2\ell+1)\, i^\ell\, e^{i\ell\pi/2}\, P_\ell(\cos\theta)}{2ik}\right]$$

let's go back to box normalization $L^{-3/2} = A$ (some constant

Compare the e^{-ikr}/r terms of approaches (i) and (ii):

$$A \sum_\ell \frac{-(2\ell+1)\, i^\ell \, e^{i\ell\pi/2} \, P_\ell(\cos\theta)}{2ik} =$$

$$\sum_\ell -A_\ell(k) \, \frac{e^{i\ell\pi/2} \, e^{-i\delta_\ell(k)}}{2ik} \, P_\ell(\cos\theta)$$

Multiply by $P_{\ell'}(\cos\theta)$ and integrate over $d\cos\theta$:

$$\Rightarrow A_\ell(k) = (2\ell+1)\, i^\ell \, e^{i\delta_\ell(k)} \, A \qquad (*)$$

Next: Compare the e^{ikr}/r terms of approaches (i) and (ii):

$$A\left[f(k,\theta) + \sum_\ell \frac{(2\ell+1)\, i^\ell \, e^{-i\ell\pi/2} \, P_\ell(\cos\theta)}{2ik} \right]$$

$$= \sum_\ell \underset{\substack{\Vert \\ (2\ell+1)\, i^\ell \, e^{i\delta_\ell(k)} A}}{A_\ell(k)} \, \frac{e^{-i\ell\pi/2} \, e^{i\delta_\ell(k)}}{2ik} \, P_\ell(\cos\theta)$$

$$\Rightarrow f(k,\theta) = \frac{1}{k} \sum_\ell (2\ell+1)\, \cancel{i^\ell} \, \underbrace{\frac{1}{2i}\left(e^{2i\delta_\ell(k)} - 1\right)}_{e^{i\delta_\ell(k)} \sin(\delta_\ell(k))} \, e^{-i\ell\pi/2} \, P_\ell(\cos\theta)$$

$$i^\ell = e^{i\ell\pi/2}$$

$$\boxed{f(k,\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\delta_\ell(k)} \sin(\delta_\ell(k))\, P_\ell(\cos\theta)} \qquad (6.4.40)$$

In practice, one typically does not have to go to $l = \infty$.

Why? Classically, $l = \underbrace{m v}_{} r$

small velocity $\Rightarrow$ small angular momentum

Thus, we expect that we will only need a finite number of partial waves, especially when we are in the low energy regime.

$f(k, \theta)$ is given in terms of an infinite number of parameters, namely the $\underbrace{\delta_l(k)}_{}$

phase shift of l's partial wave (each $\delta_l(k)$ is obtained by solving one-dimensional radial equation for given potential and given scattering energy)

To visualize this approach, let's look at the 1D case.

Approach (i):

(this is equivalent to solving radial eq. in 3D)

even parity solution: ψ_{even}

odd parity solution: ψ_{odd}

$$\psi_{even} \propto \sin(k|z|) - \tan(\delta_e(k))\cos(kz)$$

$$\propto \sin(k|z| + \delta_e(k))$$

$$\psi_{odd} \propto \frac{z}{|z|}\sin(kz) - \tan(\delta_o(k))\frac{z}{|z|}\cos(kz)$$

$$\propto \frac{z}{|z|}\sin(k|z| + \delta_o(k))$$

even/odd partial waves

Approach (ii):

incoming + reflected

$e^{ikz} + f(k)e^{-ikz}$

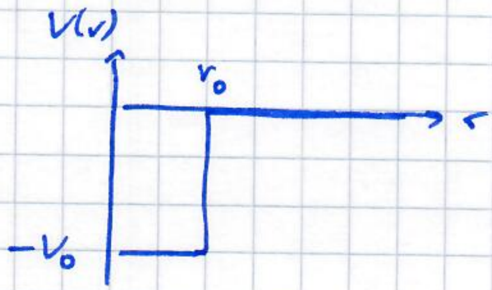
transmitted : $t(k)e^{ikz}$

Connect the two approaches by taking the wave fcts from (i) and decompose them into e^{ikz} and e^{-ikz} for $|z| > z_0$.

Note: $\delta_e(k)$ and $\delta_o(k)$ need to be calculated by solving the SE

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V(z)\right)\psi_{even/odd}(z) = E\,\psi_{even/odd}(z)$$

Let's look at the 3D SW potential:



$V_0 > 0$

$r_0 > 0$

define: $K = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$

We know: $R_e^{in}(r) = D_e(k)\, j_e(Kr)$ for $r < r_0$

$$R_e^{out}(r) = B_e(k)\left[j_e(kr) - \tan(\delta_e(k))\, n_e(kr)\right]$$

for $r > r_0$

Match logarithmic derivative at $r = r_0$:

$$\underbrace{\frac{\frac{\partial}{\partial r} R_\ell^{out}(r)\Big|_{r=r_0}}{R_\ell^{out}(r_0)}}_{\mathcal{L}_\ell^{out}(r_0)} = \underbrace{\frac{\frac{\partial}{\partial r} R_\ell^{in}(r)\Big|_{r=r_0}}{R_\ell^{in}(r)}}_{\mathcal{L}_\ell^{in}(r_0)}$$

$$\Rightarrow \mathcal{L}_\ell^{in}(r_0) = \frac{\left(\frac{\partial}{\partial r} j_\ell(kr)\right)_{r_0} - \tan(\delta_\ell(k))\left(\frac{\partial}{\partial r} n_\ell(kr)\right)_{r_0}}{j_\ell(kr_0) - \tan(\delta_\ell(k))\, n_\ell(kr_0)}$$

Solve for $\tan(\delta_\ell(k))$:

$$\boxed{\tan(\delta_\ell(k)) = \frac{\frac{\partial}{\partial r} j_\ell(kr)\Big|_{r_0} - \mathcal{L}_\ell^{in}(r_0)\, j_\ell(kr_0)}{\frac{\partial}{\partial r} n_\ell(kr)\Big|_{r_0} - \mathcal{L}_\ell^{in}(r_0)\, n_\ell(kr_0)}}$$

this equation is valid for any central potential that falls off sufficiently fast (and r_0 is chosen to be sufficiently large)

Now: apply this to SW potential.

$$\mathcal{L}_\ell^{in}(r_0) = \frac{\frac{\partial}{\partial r} j_\ell(Kr)}{j_\ell(Kr)}\Bigg|_{r_0}$$

If we know the inner solution, we get the phase shifts by matching to the (agreed upon) asymptotic boundary condition.

Specifically:

$$l=0: \quad \tan\delta_0(k) = \frac{k\cos(kr_0) - K\cot(Kr_0)\sin(kr_0)}{k\sin(kr_0) + K\cot(Kr_0)\cos(kr_0)}$$

Rearrange:

$$-\frac{\tan\delta_0(k)}{k} = \frac{-\cos(kr_0) + \frac{K}{k}\cot(Kr_0)\sin(kr_0)}{k\sin(kr_0) + K\cot(Kr_0)\cos(kr_0)}$$

If we take the $k\to 0$ limit, the r.h.s. goes to a constant.

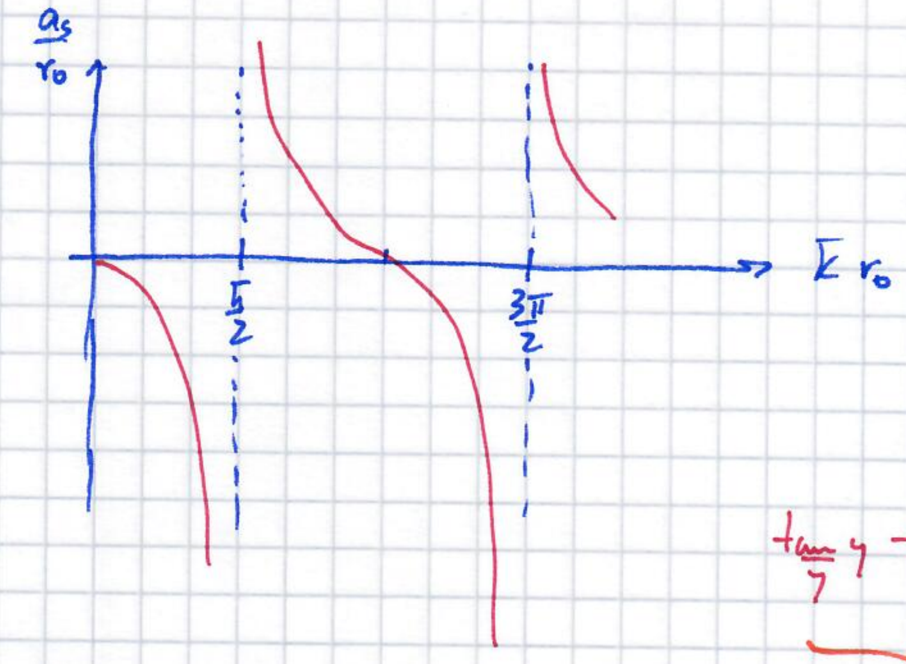
$$\lim_{k\to 0} -\frac{\tan(\delta_0(k))}{k} = r_0\left(1 - \frac{\tan(\bar{K}r_0)}{\bar{K}r_0}\right)$$

where $\bar{K} = \sqrt{\frac{2mV_0}{\hbar^2}}$

The quantity $\lim_{k\to 0} -\frac{\tan(\delta_0(k))}{k}$

is called s-wave scattering length a_s.

For SW pot.: $\frac{a_s}{r_0} = 1 - \frac{\tan y}{y}$ where $y = \bar{K}r_0$



$\tan y \to \infty$ for $y = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots$

this is exactly the condition for a new zero-energy s-wave bound state being supported by the SW potential.

Try to get a pictorial / physical understanding of the s-wave phase shift!

For this, let us look at the outside solution:

$$\sin(kr + \delta_0(k)) \propto \sin(kr) + \tan(\delta_0(k))\cos(kr)$$

$$\xrightarrow[kr \to 0]{} kr - \lim_{k\to 0} \tan(\delta_0(k))$$

$$\longrightarrow r - \lim_{k \to 0} \frac{-\tan \delta_0(k)}{k}$$

$$\longrightarrow r - a_s$$

So: in the low-energy limit,

$\sin(kr + \delta_0(k))$ goes to zero at

$r = a_s$.

Let's assume: $\delta_0(k)$ is small and positive

effective attraction

$\Rightarrow -\frac{\tan(\delta_0(k))}{k} \approx -\frac{\delta_0(k)}{k}$ = negative

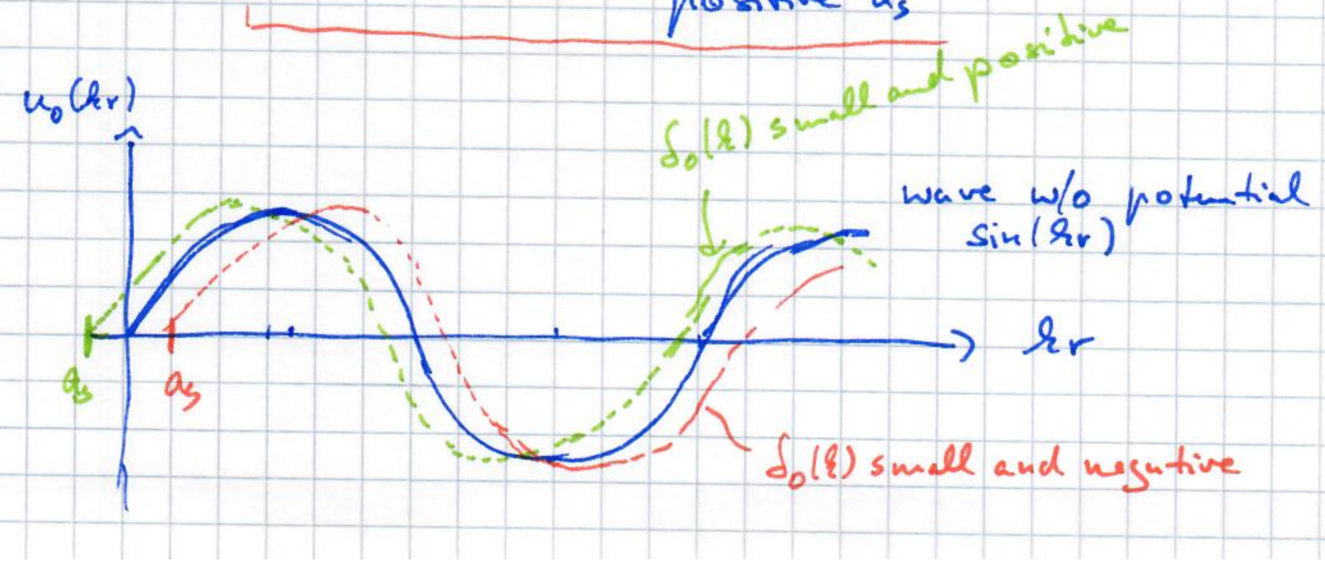
small positive $\delta_0(k) \Rightarrow$ negative a_s

Let's assume: $\delta_0(k)$ is small and negative

effective repulsion

$\Rightarrow -\frac{\tan(\delta_0(k))}{k} = -\frac{\delta_0(k)}{k}$ = positive

small negative $\delta_0(k) \Rightarrow$ positive a_s



In the sketch, we assumed that the outer solution extends into the inner region. It doesn't: for realistic systems, the inner solution looks different. We "simply" pretend that the outer solution would extend into the inner region and, by doing so, we obtain a nice geometrical interpretation of the s-wave scattering length.

What happens when a_s is very large?

Again: let's look at outside solution

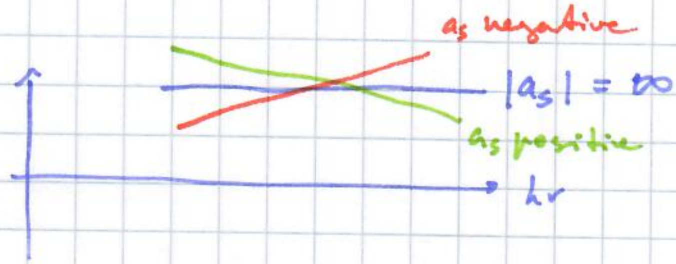
$$\sin(kr + \delta_0(k)) \longrightarrow -\left(\frac{-r}{a_s} + 1\right)$$

$$\overset{\propto}{\longrightarrow} 1 \text{ as } a_s \to \pm\infty$$

The outside wave fct is constant

→ just short of supporting a bound st. if $a_s \to -\infty$

→ just short of loosing a b. st. if $a_s \longrightarrow +\infty$



a_s negative
$|a_s| = \infty$
a_s positive
kr

Let's go back to (6.4.40) [see page 6-43]:

$$f(k,\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell(k)} \sin(\delta_\ell(k))\, P_\ell(\cos\theta)$$

Defining partial wave amplitude $f_\ell(k)$:

$$\underbrace{f_\ell(k) = \frac{2\ell+1}{k} e^{i\delta_\ell(k)} \sin(\delta_\ell(k))}$$

Note: no θ-dependence

$$\Rightarrow f(k,\theta) = \sum_{\ell=0}^{\infty} f_\ell(k)\, P_\ell(\cos\theta)$$

Recall:

$$\frac{d\sigma}{d\Omega} = |f(k,\theta)|^2$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{1}{k^2} \sum_{\ell,\ell'} (2\ell+1)(2\ell'+1)\, e^{i[\delta_\ell(k) - \delta_{\ell'}(k)]} \sin(\delta_\ell(k)) \sin(\delta_{\ell'}(k))$$

plugging in for f

$$\times P_\ell(\cos\theta)\, P_{\ell'}(\cos\theta)$$

Let's calculate the total cross section σ_{tot}:

$$\sigma_{tot} = 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega} \underbrace{\sin\theta\, d\theta}_{d\cos\theta}$$

The Legendre polynomials form a complete set => we only get a contribution when $l = l'$

$$\Rightarrow \boxed{\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l(k))}$$

In the low-energy limit:

$$\lim_{k \to 0} \sigma_{tot} \longrightarrow 4\pi a_s^2$$

In writing the scattering amplitude, we used

$$\frac{1}{2i}\left(e^{2i\delta_l(k)} - 1\right) = e^{i\delta_l(k)} \sin(\delta_l(k))$$

an aside (used below)

We can write the large r behavior of $u_l(r)$ in a variety of ways (in the equations below, the normalization factor is excluded — in fact, I'm changing it as I go along...):

$$u_\ell(k,r) \longrightarrow \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)$$

$$\longrightarrow \sin\left(kr - \frac{\ell\pi}{2}\right) + \underbrace{\tan(\delta_\ell(k))}_{K_\ell(k)} \cos\left(kr - \frac{\ell\pi}{2}\right)$$

$$\longrightarrow e^{-i(kr - \frac{\ell\pi}{2})} - \underbrace{e^{2i\delta_\ell(k)}}_{S_\ell(k)} e^{i(kr - \frac{\ell\pi}{2})}$$

But we also have:

$$\psi^{(+)}(\vec{r}) \longrightarrow e^{ikz} + \underbrace{f(k,\theta)}_{\sum_\ell (2\ell+1) \frac{1}{2i} \left(e^{2i\delta_\ell(k)} - 1\right) P_\ell(\cos\theta)} \frac{e^{ikr}}{r}$$

$$\to e^{ikz} + \sum_\ell (2\ell+1) \frac{1}{2i} \underbrace{\left(e^{2i\delta_\ell(k)} - 1\right)}_{T_\ell(k)} P_\ell(\cos\theta) \frac{e^{ikr}}{r}$$

So: K-matrix element $K_\ell(k)$

S-matrix element $S_\ell(k)$

T-matrix element $T_\ell(k)$

$$K_\ell(k) = \tan(\delta_\ell(k))$$

$$S_\ell(k) = \frac{1 + i K_\ell(k)}{1 - i K_\ell(k)}$$

$$T_\ell(k) = S_\ell(k) - 1 = \exp[2i\delta_\ell(k)] - 1$$

What does it mean to have a pole in the S-matrix $S_\ell(k)$?

Look at $u_\ell(k,r) \xrightarrow[kr \gg 1]{} e^{-i(kr - \frac{\ell\pi}{2})} - S_\ell(k) e^{i(kr - \frac{\ell\pi}{2})}$

Let $\underbrace{k \text{ be } i k^*}_{\text{we've looking at bound state}}$ with k^* real and positive

$S_\ell(k)$ has a pole $\rightarrow$ $S_\ell(k)$ blows up. Let's rewrite $u_\ell(k,r)$:

$$u_\ell(k,r) \longrightarrow \frac{1}{S_\ell(k)} e^{-i(kr - \frac{\ell\pi}{2})} - e^{i(kr - \frac{\ell\pi}{2})}$$

again, I'm changing normalization factor

goes to zero when $S_\ell(k)$ has a pole at certain negative energy

e^{ikr} falls off exponentially fall $k \to ik^*$

A pole in the S-matrix $S_\ell(k)$ corresponds to a bound state wave function.

When do we have pole in $S_\ell(k)$?

$$S_\ell(k) = \frac{1 + iK_\ell(k)}{1 - iK_\ell(k)}$$

$$\rightsquigarrow \text{pole if } \quad 1 - iK_\ell(k) = 0$$

$$\Rightarrow \quad 1 = i \tan(\delta_\ell(k))$$

$$\Rightarrow \boxed{-i = \tan(\delta_\ell(k))}$$

this is the condition for a bound state

Aside: on the HW, start with $\sin(kr - \frac{\ell\pi}{2}) + \tan(\delta_\ell(k))\cos(kr - \frac{\ell\pi}{2})$ and show how the b.st. condition follows

So: we have established a connection between scattering states and bound states.

for spherically symmetric potential, T matrix is diagonal

Also: we established a connection between "T" introduced at the beginning of this chapter and $\delta_\ell(k)$.