

Lecture 8

II.1 Two-body scattering problem

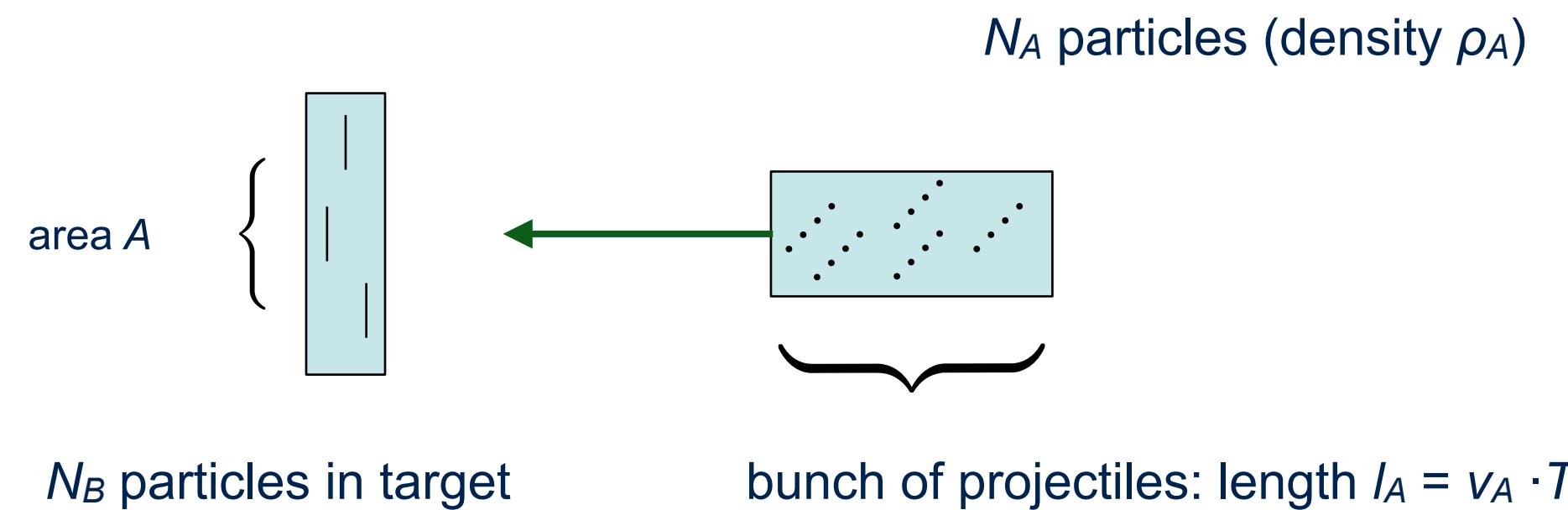
We now turn to the scattering problem. In these lecture, we will briefly introduce the underlying equations.

We will again use momentum space, which allows one directly include the boundary conditions into the resulting integral equation.

Technically, the main complication is the treatment of singularities of the integral equations.
The implementation of this technique will be part of exercise 7.

The final observable that needs to be calculate will be the **cross section**.

A sketch of a typical scattering experiment



$$\sigma = \frac{\# \text{ of events}}{T} \frac{1}{N_B} \underbrace{\frac{1}{\rho_A v_A}}_{\text{particle current } j_A} = \underbrace{\frac{\# \text{ of events}}{T}}_{\text{transition probability per unit time}} \frac{1}{j_A}$$

"in" and "out" states

In order to get the cross section, we need to calculate the transition probability per unit time. The key for this is the definition of so called "in" and "out" states.

Let us start at large negative times $T \rightarrow -\infty$. Particles are still well separated from each other, the time dependence is given by the free Hamiltonian and states are most efficiently expressed in terms of momentum eigenstates (corresponding to beam momentum)

$$\text{"initial" state} \rightarrow | i \rangle = \int d^3k_1 d^3k_2 f(\vec{k}_1) \tilde{f}(\vec{k}_2) | \vec{k}_1 \vec{k}_2 \rangle$$

Formally, the time dependence is still driven by the full Hamiltonian: $i \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$ and

$$|\Psi(t)\rangle = \exp(-i \hat{H} t) |\Psi(0)\rangle \equiv \hat{U}(t) |\Psi(0)\rangle$$

We will use here $\hat{H} = \hat{H}_0 + \hat{V}$ and $\hat{U}_0(t)$ for the time evolution operator only involving the kinetic energy.

The aim is to define a scattering state $|\Psi(t)\rangle$ that corresponds to $|i\rangle$ at large negative times.

$$\hat{U}(T) |\Psi(0)\rangle \xrightarrow{T \rightarrow -\infty} \hat{U}_0(T) |i\rangle$$

This idea defines "in" and "out" states:

$$|i, in\rangle \equiv \underbrace{\lim_{T \rightarrow -\infty} \hat{U}^\dagger(T) \hat{U}_0(T)}_{\Omega_+ - \text{M}\ddot{\text{o}}\text{l}\text{l}\text{er operator}} |i\rangle$$

$$|f, out\rangle \equiv \underbrace{\lim_{T \rightarrow \infty} \hat{U}^\dagger(T) \hat{U}_0(T)}_{\Omega_- - \text{M}\ddot{\text{o}}\text{l}\text{l}\text{er operator}} |f\rangle$$

↑ "final" state

S matrix

Given the "in" and "out" states, the transition probability from an "initial" to "final" state is given by the S operator (or in momentum space) S matrix

$$\underbrace{|\langle f, \text{out} | i, \text{in} \rangle|^2}_{S_{fi}} = |\langle f | \underbrace{\Omega_-^\dagger \Omega_+}_{\text{S operator}} | i \rangle|^2$$

(scattering) matrix

Trick to perform limits in time $T \rightarrow \pm \infty$:

$$\lim_{T \rightarrow -\infty} f(T) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 dt \exp(\varepsilon t) f(t)$$

$$\lim_{T \rightarrow \infty} f(T) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^\infty dt \exp(-\varepsilon t) f(t)$$

This trick allows to rewrite the Möller operator in a time-independent form

$$| i, \text{in} \rangle = \lim_{T \rightarrow -\infty} \hat{U}^\dagger(T) \hat{U}_0(T) | i \rangle = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 dt \exp(\varepsilon t) \hat{U}^\dagger(t) \hat{U}_0(t) | i \rangle$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^0 dt \exp(\varepsilon t) \exp(+i\hat{H}t) \exp(-i\hat{H}_0 t) \int d^3 k_1 d^3 k_2 f(\vec{k}_1) \tilde{f}(\vec{k}_2) | \vec{k}_1 \vec{k}_2 \rangle = \int d^3 k_1 d^3 k_2 f(\vec{k}_1) \tilde{f}(\vec{k}_2) \underbrace{\lim_{\varepsilon \rightarrow 0^+} \frac{i\varepsilon}{E_{k_1 k_2} + i\varepsilon - \hat{H}} | \vec{k}_1 \vec{k}_2 \rangle}_{\equiv | \vec{k}_1 \vec{k}_2 \rangle^{(+)}}$$

The calculation of these "in" states is a **time-independent problem!**

"in" state of $| \vec{k}_1 \vec{k}_2 \rangle$

Analogously, one finds

$$| f, \text{out} \rangle = \int d^3k_1 d^3k_2 f(\vec{k}_1) \tilde{f}(\vec{k}_2) \underbrace{\lim_{\epsilon \rightarrow 0^+} \frac{-i\epsilon}{E_{k_1 k_2} - i\epsilon - \hat{H}}}_{\equiv |\vec{k}_1 \vec{k}_2 \rangle^{(-)}} | \vec{k}_1 \vec{k}_2 \rangle$$

“out” state of $|\vec{k}_1 \vec{k}_2 \rangle$

So the problem of finding “in” and “out” states is driven by **resolvent operators**

$$\hat{G}^{(\pm)} \equiv \frac{1}{E_{k_1 k_2} \pm i\epsilon - \hat{H}}$$

and will now be interested in expressing the S-matrix ${}^{(-)}\langle \vec{k}'_1 \vec{k}'_2 | \vec{k}_1 \vec{k}_2 \rangle^{(+)}$ in terms of $\hat{G}^{(\pm)}$

Using **translation invariance**, the operator conserves total momentum. Therefore, we can immediately express the problem in terms of **relative coordinates** $S_{fi} = {}^{(-)}\langle \vec{p}' | \vec{p} \rangle^{(+)}$ and

$$\hat{G}^{(\pm)} \equiv \frac{1}{E_p \pm i\epsilon - \hat{H}} \quad \text{or more generally} \quad \hat{G}^{(\pm)}(E) \equiv \frac{1}{E \pm i\epsilon - \hat{H}} \quad \text{and} \quad \hat{G}_0^{(\pm)}(E) \equiv \frac{1}{E \pm i\epsilon - \hat{H}_0}$$

With some algebra, it is straight forward to show that

$$G^{(\pm)}(E) = G_0^{(\pm)}(E) + G^{(\pm)}(E) \quad V \quad G_0^{(\pm)}(E) = G_0^{(\pm)}(E) + G_0^{(\pm)}(E) \quad V \quad G^{(\pm)}(E)$$

This **resolvent identity** has some important consequences making the solution later on more easy.

1) Lippmann-Schwinger equation for the "in" and "out" states

$$|\vec{p}\rangle^{(\pm)} = \frac{\pm i\varepsilon}{E_p \pm i\varepsilon - H} |\vec{p}\rangle = \underbrace{\frac{\pm i\varepsilon}{E_p \pm i\varepsilon - H_0} |\vec{p}\rangle}_{=|\vec{p}\rangle} + \frac{1}{E_p \pm i\varepsilon - H_0} V \underbrace{\frac{\pm i\varepsilon}{E_p \pm i\varepsilon - H} |\vec{p}\rangle}_{=|\vec{p}\rangle^{(\pm)}}$$

2) Formal solution in terms of the resolvent

- a. "in" and "out" states are eigenstates of \hat{H}

$$(E_p - H) |\vec{p}\rangle^{(\pm)} = 0$$

b.

$$|\vec{p}\rangle^{(\pm)} = \frac{\pm i\varepsilon}{E_p \pm i\varepsilon - H} |\vec{p}\rangle = \underbrace{\frac{\pm i\varepsilon}{E_p \pm i\varepsilon - H_0} |\vec{p}\rangle}_{=|\vec{p}\rangle} + \frac{1}{E_p \pm i\varepsilon - H} V \underbrace{\frac{\pm i\varepsilon}{E_p \pm i\varepsilon - H_0} |\vec{p}\rangle}_{=|\vec{p}\rangle}$$

and

$${}^{(\pm)}\langle \vec{p}| = \langle \vec{p}| + \langle \vec{p}| V \frac{1}{E_p \mp i\varepsilon - H}$$



Note the sign change!

3) Introduction of the t-matrix

$$\begin{aligned} {}^{(-)}\langle \vec{p}' | \vec{p}\rangle^{(+)} &= \langle \vec{p}' | \vec{p}\rangle^{(+)} + \langle \vec{p}' | V \frac{1}{E_{p'} + i\varepsilon - H} |\vec{p}\rangle^{(+)} && \text{use relation 2b)} \\ &= \langle \vec{p}' | \vec{p}\rangle + \langle \vec{p}' | \frac{1}{E_p + i\varepsilon - H_0} V |\vec{p}\rangle^{(+)} + \langle \vec{p}' | V \frac{1}{E_{p'} + i\varepsilon - H} |\vec{p}\rangle^{(+)} && \text{use Lippmann-Schwinger equation} \\ &= \delta^{(3)}(\vec{p} - \vec{p}') + \underbrace{\left(\frac{1}{E_{p'} + i\varepsilon - E_p} + \frac{1}{E_p + i\varepsilon - E_{p'}} \right)}_{=-2\pi i \delta(E_p - E_{p'})} \underbrace{\langle \vec{p}' | V |\vec{p}\rangle^{(+)}}_{\equiv t(\vec{p}', \vec{p})} && \text{use eigenstates of } \hat{H}_0 \text{ and } \hat{H} \end{aligned}$$

We justify the δ -function on the last line on the next slide.

This relates the S-matrix to t-matrix, which is a smooth function and can be numerically calculated!

The t-matrix can be directly used to get the cross section $d\sigma = (2\pi)^4 \delta(E_{p'} - E_p) \frac{1}{v_A} |t(\vec{p}', \vec{p})|^2$

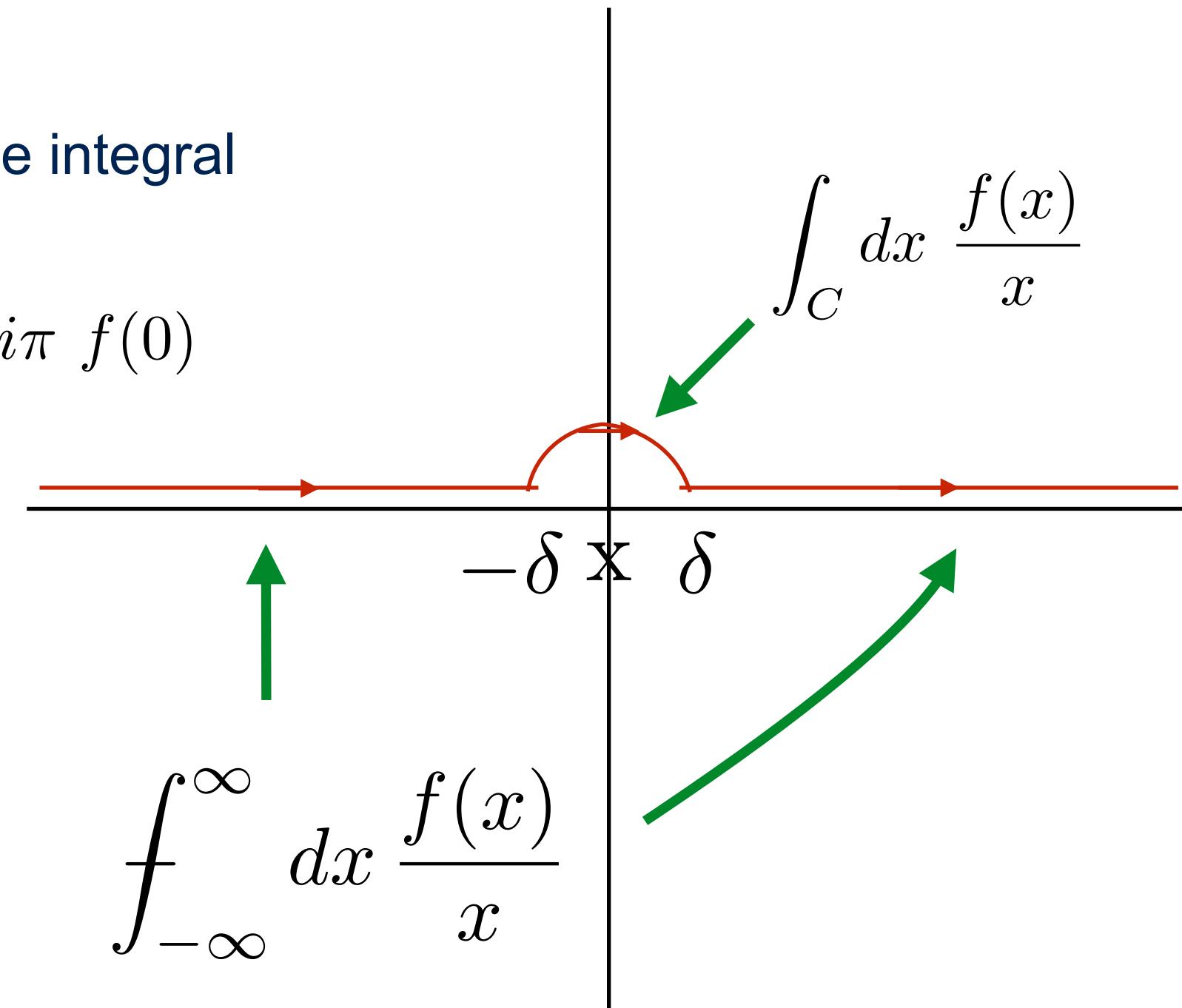
Treatment of the ε limits by integration in the complex plane

$$\int_{-\infty}^{\infty} dx \frac{f(x)}{x + i\varepsilon} = \text{P.V.} \int_{-\infty}^{\infty} dx \frac{f(x)}{x} - i\pi \int_{-\infty}^{\infty} dx f(x) \delta(x) = \text{P.V.} \int_{-\infty}^{\infty} dx \frac{f(x)}{x} - i\pi f(0)$$

principal value integral

or in shorter notation

$$\frac{1}{x + i\varepsilon} = \text{P.V.} \frac{1}{x} - i\pi\delta(x)$$



$$\int_C dx \frac{f(x)}{x} = \int_{\pi}^0 d\varphi \frac{i\delta \exp(i\varphi)}{\delta \exp(i\varphi)} f(\delta \exp(i\varphi)) = -i\pi f(0) \quad \checkmark$$

This relation was used to introduce the t-matrix and will be very important to implement the solution later on.

The t-matrix can be directly obtained using the Lippmann-Schwinger equation for the t-matrix

$$t(\vec{p}', \vec{p}) = \langle \vec{p}' | V | \vec{p} \rangle^{(+)} = \langle \vec{p}' | V | \vec{p} \rangle + \langle \vec{p}' | V \frac{1}{E_p + i\epsilon - H_0} V | \vec{p} \rangle^{(+)}$$

or

$$t(\vec{p}', \vec{p}) = V(\vec{p}', \vec{p}) + \int d^3 p'' V(\vec{p}', \vec{p}'') \frac{1}{E_p + i\epsilon - E_{p''}} t(\vec{p}'', \vec{p})$$

energy “parameter” E

For the scattering observables only the **on-shell t-matrix** ($E = E_{p'} = E_p$) is required.

Note that the solution also requires the **half-off shell t-matrix** $t(\vec{p}'', \vec{p})$ for $E = E_p = p^2/(2\mu)$.

Later, we will need the **fully off-shell t-matrix** ($E \neq E_p$) for the solution of the three-body problem.

The t-matrix can also be expanded in terms of **partial waves**. Angular momentum conservation directly carries over to the t-matrix.

One finds

$$t_l(p', p) = V_l(p', p) + \int dp'' p''^2 V_l(p', p'') \frac{1}{E_p + i\epsilon - E_{p''}} t_l(p'', p)$$

This is the central equation for numerical solutions of the scattering problem.

A few side remarks that are useful for solving, checking the result or representation of the results

1) explicit treatment of ε (formulated for a general energy $E_q = q^2/(2\mu)$)

$$\begin{aligned}
 t_l(p', p) &= V_l(p', p) + \int_0^\infty dp'' p''^2 V_l(p', p'') \frac{1}{E_q + i\varepsilon - E_{p''}} t_l(p'', p) = V_l(p', p) + \oint_0^\infty dp'' p''^2 V_l(p', p'') \frac{1}{E_q - E_{p''}} t_l(p'', p) - i\pi \int_0^\infty dp'' p''^2 V_l(p', p'') \delta(E_q - E_{p''}) t_l(p'', p) \\
 &= V_l(p', p) + \oint_0^\infty dp'' p''^2 V_l(p', p'') \frac{1}{E_q - E_{p''}} t_l(p'', p) - i\pi q\mu V_l(p', q) t_l(q, p) \\
 &= V_l(p', p) + \oint_0^\infty dp'' \frac{p''^2 V_l(p', p'') t_l(p'', p) - q^2 V_l(p', q) t_l(q, p)}{E_q - E_{p''}} + \oint_0^\infty dp'' \frac{q^2 V_l(p', q) t_l(q, p)}{E_q - E_{p''}} - i\pi q\mu V_l(p', q) t_l(q, p) \\
 &= V_l(p', p) + \int_0^\infty dp'' \frac{2\mu p''^2 V_l(p', p'') t_l(p'', p) - 2\mu q^2 V_l(p', q) t_l(q, p)}{q^2 - p''^2} + 2\mu q^2 V_l(p', q) t_l(q, p) \oint_0^\infty dp'' \frac{1}{q^2 - p''^2} - i\pi q\mu V_l(p', q) t_l(q, p)
 \end{aligned}$$

it is useful to evaluate the principal value integral for a given upper bound (see exercise):

$$\oint_0^{p_{max}} dp'' \frac{1}{q^2 - p''^2} = \frac{1}{2q} \ln \left(\frac{p_{max} + q}{p_{max} - q} \right)$$

2) The S-matrix is unitary

$$S S^\dagger = \mathbb{1} \quad \text{or} \quad \int d^3 p'' \langle \vec{p}' | \vec{p}'' \rangle^{(+)} \langle \vec{p}'' | \vec{p} \rangle^{(-)} = \delta(\vec{p}' - \vec{p})$$

in a partial wave expansion

$$\langle \vec{p}' | \vec{p} \rangle^{(+)} = \frac{\delta(p - p')}{pp'} \sum_{lm} Y_{lm}^*(\hat{p}') Y_{lm}(\hat{p}) - 2\pi i \frac{\mu}{p} \delta(p - p') \sum_{lm} Y_{lm}^*(\hat{p}') t_l(p', p) Y_{lm}(\hat{p}) \equiv \frac{\delta(p - p')}{pp'} \sum_{lm} Y_{lm}^*(\hat{p}') S_l(p) Y_{lm}(\hat{p})$$

where $S_l(p) = 1 - 2\pi i \mu p t_l(p, p)$.

The unitarity implies $|S_l(p)|^2 = 1$.

Based on this property it is possible to quantify the S- and t-matrix by a real phase shift $\delta_l(p)$:

$$S_l(p) = \exp(2i\delta_l(p)) \quad \text{and} \quad t_l(p, p) = -\frac{\sin \delta_l(p)}{\pi \mu p} \exp(i\delta_l(p))$$

It will be an exercise to develop the code to obtain the t-matrix, phase shifts and cross sections