Lecture 10

II.4 Faddeev equations for 3-body scattering

In this lecture, we will formulate the equations to obtain a 3-body scattering state and rewrite them into a form that allows the numerical solution and the extraction of observables (cross sections).

An example implementation will be provided as Jupyter notebook.

We again consider a system of three identical spinless bosons.

The problem has exactly one s-wave (l=0) bound two-body bound state and asymptotic incoming state is a two-body bound state scattering on the third particle with a relative momentum $\vec{q}_0 = q_0 \, \hat{e}_z$.

The corresponding incoming state is

$$| \, b \, \rangle \equiv | \, \varphi_{12} \, \vec{q}_0 \, \rangle \text{ or } | \, \varphi_{23} \, \vec{q}_0 \, \rangle \text{ or } | \, \varphi_{31} \, \vec{q}_0 \, \rangle$$

we will also (for outgoing states) require an asymptotic state of three non-interacting particles

$$| \, a \, \rangle \equiv | \, \vec{p}_0 \, \vec{q}_0 \, \rangle$$

Define "in" and "out" states

Similar to the two-body scattering problem, we can now define "in"- and "out"-states corresponding to $|\, a \,\rangle$ and $|\, b \,\rangle$, i.e.

$$|\, b \,\rangle^{(\pm)} \equiv \lim_{\varepsilon \to 0^+} \frac{\pm i\varepsilon}{E \pm i\varepsilon - H} \,|\, b \,\rangle$$

and similar for $|\, a \,\rangle$.

The Pauli principle requires symmetric states. Assuming that the the two-body subsystem is already symmetrized (only even angular momenta l!), the symmetrizer only requires three parts

$$\left\{ |\, b \,\rangle \right\} = \frac{1}{\sqrt{3}} \,(1 + P)\,|\, b \,\rangle$$

This directly translates to the scattering states

$$\left\{ |\, b \,\rangle^{(\pm)} \right\} = \frac{\pm i\varepsilon}{E \pm i\varepsilon - H} \, \left\{ |\, b \,\rangle \right\}$$ (limes $\varepsilon \to 0^+$ is implied as usual)

Definition of the S-matrix and scattering amplitude

Based on the "in"- and "out"-states, we can define the S-matrix and read off the scattering amplitude.
Note that we have two possible cases:

1) breakup scattering

$$S_{ab} = \left\{ {}^{(-)}\langle a \,|\, \right\} \left\{ \,|\, b \,\rangle^{(+)} \right\} = {}^{(-)}\langle a \,|\, (1+P) \,|\, b \,\rangle^{(+)}$$ (note cancelation of factor 3)

We need to use the relation

$$|\, a \,\rangle^{(\pm)} = \frac{\pm i\varepsilon}{E \pm i\varepsilon - H} \,|\, a \,\rangle = |\, a \,\rangle + \frac{1}{E \pm i\varepsilon - H} \left(V_{12} + V_{23} + V_{31} \right) \,|\, a \,\rangle$$

or

$$|\, a \,\rangle^{(-)} - |\, a \,\rangle^{(+)} = 2\pi i \; \delta(E - H) \; \left(V_{12} + V_{23} + V_{31} \right) \;|\, a \,\rangle$$

to again derive the standard relation of the scattering amplitude (t-matrix) and S-matrix (for breakup)

$$S_{ab} = {}^{(+)}\langle a \,|\, (1+P) \,|\, b \,\rangle^{(+)} - 2\pi i \; \delta(E_b - E_a) \; \underbrace{\langle a \,|\, \left(V_{12} + V_{23} + V_{31} \right) \; (1+P) \;|\, b \,\rangle^{(+)}}_{M_{ab}}$$

This defines the amplitude M_{ab}.
It is straightforward to obtain the cross section for break up as (phase space integral)

$$\frac{d^5\sigma}{d\hat{p}\, d\hat{q}\, dq} = (2\pi)^4 \frac{m}{3q_0} q^2 p \,|\, M_{\vec{p}\,\vec{q},q_0} \,|^2$$

2) elastic scattering

$$S_{b'b} = \left\{ {}^{(-)}\langle\, b' \,|\, \right\} \left\{ \,|\, b \,\rangle^{(+)} \right\} = {}^{(-)} \langle\, b' \,|\, (1+P) \,|\, b \,\rangle^{(+)}$$

We need to use the relation

$$|\, b' \,\rangle^{(\pm)} = \frac{\pm i\varepsilon}{E \pm i\varepsilon - H} \,|\, b' \,\rangle = |\, b' \,\rangle + \frac{1}{E \pm i\varepsilon - H} \left(V_{23} + V_{31} \right) \,|\, b' \,\rangle$$

since

$$\frac{\pm i\varepsilon}{E_{b'} \pm i\varepsilon - H_0 - V_{12}} \,|\, b' \,\rangle = |\, b' \,\rangle$$

or

$$|\, b' \,\rangle^{(-)} - |\, b' \,\rangle^{(+)} = 2\pi i \;\delta(E - H) \left(V_{23} + V_{31} \right) \,|\, b' \,\rangle$$

to again derive the standard relation of the scattering amplitude (t-matrix) and S-matrix (for breakup)

$$S_{b'b} = {}^{(+)} \langle\, b' \,|\, (1+P) \,|\, b \,\rangle^{(+)} - 2\pi i \;\delta(E_b - E_{b'}) \underbrace{\langle\, b' \,|\, \left(V_{23} + V_{31} \right) \, (1+P) \,|\, b \,\rangle^{(+)}}_{M_{b'b}}$$

This defines the amplitude $M_{b'b}$ for elastic scattering.
It is straightforward to obtain the cross section for break up as (phase space integral)

$$\frac{d^2\sigma}{d\hat{q}} = (2\pi)^4 \frac{2m^2}{3} \,|\, M_{\vec{q}',q_0} \,|^2$$

Faddeev equations for the breakup amplitude

It is easier to formulate Faddeev equations for the break up amplitude and use the result also for elastic scattering!

We define Faddeev components of the scattering state

$$|\psi_{ij}\rangle \equiv V_{ij} \frac{i\varepsilon}{E+i\varepsilon-H}(1+P)|b\rangle \quad \text{so that} \quad |\psi_{23}\rangle + |\psi_{31}\rangle = P|\psi_{12}\rangle \quad \text{and} \quad M_{ab} = \langle a|(1+P)|\psi_{12}\rangle$$

Using the definition of the Faddeev component, we obtain

$$|\psi_{12}\rangle = V_{12}\frac{i\varepsilon}{E+i\varepsilon-H}(1+P)|b\rangle = V_{12}\frac{i\varepsilon}{E+i\varepsilon-H_0-V_{12}}(1+P)|b\rangle + V_{12}\frac{1}{E+i\varepsilon-H_0-V_{12}}(V_{23}+V_{31})\frac{i\varepsilon}{E+i\varepsilon-H}(1+P)|b\rangle$$

$$= \underbrace{V_{12}}_{E-H_0}|b\rangle + V_{12}\frac{1}{E+i\varepsilon-H_0-V_{12}}P|\psi_{12}\rangle = (E-H_0)|b\rangle + \underbrace{t_{12}\frac{1}{E+i\varepsilon-H_0}P|\psi_{12}\rangle}_{\equiv|T_{12}\rangle}$$

Note the relations:

$$V_{12}\frac{1}{E+i\varepsilon-H_0-V_{12}} = t_{12}\frac{1}{E+i\varepsilon-H_0}$$ (Lippmann-Schwinger equation for the two-body t-matrix in 3-body space)

$$\frac{i\varepsilon}{E+i\varepsilon-H_0-V_{12}}(1+P)|b\rangle = |b\rangle$$ ($P|b\rangle$ is not eigenstate of H_0+V_{12})

In order to avoid any delta-function components, we are interested in the numerical solution for $|\, T_{12} \,\rangle$

$$|\, T_{12} \,\rangle = t_{12} \frac{1}{E + i\varepsilon - H_0} P \,|\, \psi_{12} \,\rangle = t_{12} \frac{1}{E + i\varepsilon - H_0} P \, \Big((E - H_0) \,|\, b \,\rangle + |\, T_{12} \,\rangle \Big) = t_{12} \, P \,|\, b \,\rangle + t_{12} \, P \frac{1}{E + i\varepsilon - H_0} \,|\, T_{12} \,\rangle$$

The last equation needs to be numerically implemented!

$|\, T_{12} \,\rangle$ directly gives the breakup and elastic amplitude!

$$M_{ab} = \langle\, a \,|\, (1 + P) \, (E_b - H_0) \,|\, b \rangle + \langle\, a \,|\, (1 + P) \,|\, T_{12} \,\rangle = \langle\, a \,|\, (1 + P) \,|\, T_{12} \,\rangle$$

$$M_{b'b} = \langle\, b' \,|\, P \, (E_b - H_0) \,|\, b \rangle + \langle\, b' \,|\, P \,|\, T_{12} \,\rangle$$

Now we turn to the numerical implementation which requires a careful treatment of the singularities and poles.

This needs to include the singularity of the free solvent $\dfrac{1}{E + i\varepsilon - H_0}$

and also the pole of the t-matrix at two-body subsystem energies $E_{12} \approx E_d < 0$ (two-body binding energy):

$$t_{12} \approx (E_{12} - H_0) \,|\, \varphi_{12} \,\rangle \frac{1}{E_{12} + i\varepsilon - E_d} \langle\, \varphi_{12} \,|\, (E_{12} - H_0)$$

Representation in the Jacobi momentum basis

We use the same basis as for the bound state problem: $|\, p\, q\, \alpha \rangle = |\, p\, q\, (l\lambda) LM \rangle$ (often M will be dropped because of rotational invariance

We also use that $E = E_d + \dfrac{3q_0^2}{4m}$ and the matrix elements

$$\langle\, p\, q\, \alpha \,|\, b \,\rangle = \delta_{l0}\; \varphi(p)\; \frac{\delta(q - q_0)}{q\, q_0}\; Y_{\lambda 0}(\hat{q}_0)\; (\, 0\, \lambda\, L\, , 0\, 0\, M\,)$$

(z-direction of $\overrightarrow{q_0}$ breaks rotational invariance, selects $M = 0$)

and
$$\langle\, p\, q\, \alpha \,|\, t_{12} \,|\, p'\, q'\, \alpha' \,\rangle = t_l\left(p, p'; E - \frac{3q^2}{4m}\right) \delta_{\alpha\alpha'} \frac{\delta(q - q')}{q\, q'} \equiv \frac{\tilde{t}_l\left(p, p'; E - \frac{3q^2}{4m}\right)}{E_d + \frac{3q_0^2}{4m} + i\varepsilon - \frac{3q^2}{4m} - E_d} \delta_{\alpha\alpha'} \frac{\delta(q - q')}{q\, q'}$$

and write down the Faddeev equation using $\left(\dfrac{3q_0^2}{4m} + i\varepsilon - \dfrac{3q^2}{4m}\right) \langle\, p\, q\, \alpha \,|\, T_{12} \,\rangle = \tilde{T}_\alpha(pq)$

$$\langle\, p\, q\, \alpha \,|\, T_{12} \,\rangle = \sum_{\alpha''} \int dp'' p''^2 dq'' q''^2\; \langle\, p\, q\, \alpha \,|\, t_{12}\; P\; |\, p''\, q''\, \alpha'' \,\rangle \langle\, p''\, q''\, \alpha'' \,|\, b \,\rangle$$

$$+ \sum_{\alpha''} \int dp'' p''^2 dq'' q''^2\; \langle\, p\, q\, \alpha \,|\, t_{12}\; P\; \frac{1}{E + i\varepsilon - H_0} \,|\, p''\, q''\, \alpha'' \,\rangle \langle\, p''\, q''\, \alpha'' \,|\, T_{12} \,\rangle$$

Using $\tilde{t}_{12}$ for the t-matrix operator where the pole has been removed as above, we explicitly see all poles:

$$\tilde{T}_\alpha(pq) = \sum_{\alpha''} \int dp'' p''^2 dq'' q''^2 \, \langle\, p\, q\, \alpha \,|\, \tilde{t}_{12}\; P \;|\, p''\, q''\, \alpha'' \,\rangle \langle\, p''\, q''\, \alpha'' \,|\, b \,\rangle$$
$$+ \sum_{\alpha''} \int dp'' p''^2 dq'' q''^2 \, \langle\, p\, q\, \alpha \,|\, \tilde{t}_{12}\; P \;|\, p''\, q''\, \alpha'' \,\rangle \frac{1}{E + i\varepsilon - \frac{3q''^2}{4m} - \frac{p''^2}{m}} \frac{\tilde{T}_{\alpha''}(p''q'')}{\frac{3{q_0}^2}{4m} + i\varepsilon - \frac{3q''^2}{4m}}$$

The numerical treatment of these poles is very difficult!

The permutation operator induces angular dependence of the pole positions which cannot be avoid for both poles at the same time. Therefore, we will here use a partial fraction decomposition to separate the two poles depending on q_0:

$$\frac{1}{E + i\varepsilon - \frac{3q''^2}{4m} - \frac{p''^2}{m}} \frac{1}{\frac{3{q_0}^2}{4m} + i\varepsilon - \frac{3q''^2}{4m}} = \left(\frac{1}{\frac{3{q_0}^2}{4m} + i\varepsilon - \frac{3q''^2}{4m}} - \frac{1}{E + i\varepsilon - \frac{3q''^2}{4m} - \frac{p''^2}{m}} \right) \frac{m}{mE_d - p''^2}$$

The coefficient is independent of q_0 and does not have any singularity!

Let us for now focus on the kernel of the equation (inhomogeneity can be treated later (easier))

$$= \sum_{\alpha''} \int dp'' p''^2 dq'' q''^2 \, \langle \, p \, q \, \alpha \, | \, \tilde{t}_{12} \, P \, | p'' \, q'' \, \alpha'' \rangle \frac{1}{\frac{3q_0^2}{4m} + i\varepsilon - \frac{3q''^2}{4m}} \frac{m\tilde{T}_{\alpha''}(p''q'')}{mE_d - p''^2}$$

$$- \sum_{\alpha''} \int dp'' p''^2 dq'' q''^2 \, \langle \, p \, q \, \alpha \, | \, \tilde{t}_{12} \, P \, | p'' \, q'' \, \alpha'' \rangle \frac{1}{E + i\varepsilon - \frac{3q''^2}{4m} - \frac{p''^2}{m}} \frac{m\tilde{T}_{\alpha''}(p''q'')}{mE_d - p''^2}$$

Now the kinetic energy operator in the second term can be commuted with P. Therefore, we find

$$= \sum_{\alpha''} \int dp' p'^2 \int dp'' p''^2 dq'' q''^2 \, \tilde{t}_l \left(p, p'; E - \frac{3q^2}{4m} \right) \langle \, p' \, q \, \alpha \, | \, P \, | p'' \, q'' \, \alpha'' \rangle \frac{1}{\frac{3q_0^2}{4m} + i\varepsilon - \frac{3q''^2}{4m}} \frac{m\tilde{T}_{\alpha''}(p''q'')}{mE_d - p''^2}$$

$$- \sum_{\alpha''} \int dp' p'^2 \int dp'' p''^2 dq'' q''^2 \, \tilde{t}_l \left(p, p'; E - \frac{3q^2}{4m} \right) \frac{1}{E + i\varepsilon - \frac{3q^2}{4m} - \frac{p'^2}{m}} \langle \, p' \, q \, \alpha \, | \, P \, | p'' \, q'' \, \alpha'' \rangle \frac{m\tilde{T}_{\alpha''}(p''q'')}{mE_d - p''^2}$$

Now we use two different ways to represent the permutation operator, so that we keep the q'' integration in the first term, but the p' integration in the second term!

From the last lecture and bonus exercise, you can remind yourself that

$$\langle\, p'\, q\, \alpha \,|\, P\, |p''\, q''\, \alpha'' \rangle = \int_{-1}^{1} dx\, \frac{\delta(p' - \pi(qq''x))}{p'^2}\, \frac{\delta(p'' - \pi'(qq''x))}{p''^2}\, 2G_{\alpha\alpha''}(qq''x)$$

$$\langle\, p'\, q\, \alpha \,|\, P\, |p''\, q''\, \alpha'' \rangle = \int_{-1}^{1} dx\, \frac{\delta(p'' - \tilde{\pi}(p'qx))}{p''^2}\, \frac{\delta(q'' - \tilde{\chi}(p'qx))}{q''^2}\, 2\tilde{G}_{\alpha\alpha''}(p'qx)$$ (note the factors 2)

and use it to express the kernel in the desired way:

$$= \int dq'' \frac{1}{\frac{3q_0{}^2}{4m} + i\varepsilon - \frac{3q''^2}{4m}} \underbrace{q''^2 \int_{-1}^{1} dx\, \tilde{t}_l\left(p, \pi(qq''x); E - \frac{3q^2}{4m}\right) \sum_{\alpha''} 2G_{\alpha\alpha''}(qq''x)\, \frac{m\tilde{T}_{\alpha}(\pi'(qq''x)q'')}{mE_d - \pi'(qq''x)^2}}_{\equiv \mathscr{F}_{\alpha}(pqq'')}$$

$$- \int dp' \frac{1}{E + i\varepsilon - \frac{3q^2}{4m} - \frac{p'^2}{m}} \underbrace{p'^2\, \tilde{t}_l\left(p, p'; E - \frac{3q^2}{4m}\right) \sum_{\alpha''} \int_{-1}^{1} dx\; 2\tilde{G}_{\alpha\alpha''}(p'qx)\, \frac{m\tilde{T}_{\alpha''}(\tilde{\pi}(p'qx)\tilde{\chi}(p'qx))}{mE_d - \tilde{\pi}(p'qx)^2}}_{\mathscr{G}_{\alpha}(pp'q)}$$

Thereby the two functions $\mathscr{F}_{\alpha}$ and $\mathscr{G}_{\alpha}$ are smooth.

Now the poles can be treated the same way as in the two-body case. The kernel becomes

$$= \int dq'' \frac{\frac{4m}{3}\mathscr{F}_\alpha(pqq'')}{q_0^2 + i\varepsilon - q''^2} - \int dp' \frac{m\mathscr{G}_\alpha(pp'q)}{\underbrace{mE - \frac{3q^2}{4}}_{\equiv p_0^2(q)} + i\varepsilon - p'^2}$$

(p_0^2 can be negative!)

$$= \int_0^{q_{max}} dq'' \frac{\frac{4m}{3}\left(\mathscr{F}_\alpha(pqq'') - \mathscr{F}_\alpha(pqq_0)\right)}{q_0^2 + i\varepsilon - q''^2} + \left[\ln\left(\frac{q_{max}+q_0}{q_{max}-q_0}\right) - i\pi\right]\frac{4m}{6q_0}\mathscr{F}_\alpha(pqq_0) - \int_0^{p_{max}} dp' \frac{m\left(\mathscr{G}_\alpha(pp'q) - \mathscr{G}_\alpha(pp_0q)\right)}{\underbrace{mE - \frac{3q^2}{4}}_{\equiv p_0^2(q)} + i\varepsilon - p'^2} - \left[\ln\left(\frac{p_{max}+p_0}{p_{max}-p_0}\right) - i\pi\right]\frac{m}{2p_0}\mathscr{G}_\alpha(pp_0q)$$

where the terms related to p_0 only contribute for $p_0^2 > 0$.

In this form the 3-body scattering equation can be discretized.
We set up equations for $T_\alpha(p_i q_j)$ for $i = 0,\ldots,N_p - 1$ and $j = 0,\ldots,N_q$ where $q_{N_q} = q_0$.

Using the usual spline interpolation

$$f(p) = \sum_{m=0}^{N_p-1} S_m(p) f(p_m) \quad \text{and} \quad f(q) = \sum_{n=0}^{N_q-1} \tilde{S}_n(q) f(q_n)$$

the discretized kernel can be written in terms of the first and second part as

$$\mathscr{K}_{\alpha\alpha''}(p_i q_j, p_m q_l) = \mathscr{K}^{(1)}_{\alpha\alpha''}(p_i q_j, p_m q_l) + \mathscr{K}^{(2)}_{\alpha\alpha''}(p_i q_j, p_m q_l)$$

The two parts are given by

$$\mathcal{K}^{(1)}_{\alpha\alpha''}(p_i q_j, p_m q_l) = \begin{cases} \omega_l^q \dfrac{\frac{4m}{3}\mathcal{F}^m_{\alpha\alpha''}(p_i q_j q_l)}{q_0{}^2 + i\varepsilon - q_l{}^2} & l \neq N_q \\ \left[\dfrac{1}{2q_0}\ln\left(\dfrac{q_{max}+q_0}{q_{max}-q_0}\right) - i\pi\dfrac{1}{2q_0} - \sum_{\tilde{l}=0}^{N_q-1}\omega_{\tilde{l}}^q \dfrac{1}{q_0{}^2 + i\varepsilon - q_{\tilde{l}}{}^2}\right]\dfrac{4m}{3}\mathcal{F}^m_{\alpha\alpha''}(p_i q_j q_0) & l = N_q \end{cases}$$

and

$$\mathcal{K}^{(2)}_{\alpha\alpha''}(p_i q_j, p_m q_l) = -\sum_{n=0}^{N_p-1}\omega_n^p \frac{m\mathcal{G}^{ml}_{\alpha}(p_i p_n q_j)}{p_0^2(q_j) + i\varepsilon - p_n{}^2} - \left[\frac{1}{2p_0}\left(\ln\left(\frac{p_{max}+p_0}{p_{max}-p_0}\right) - i\pi\right) - \sum_{n=0}^{N_p-1}\omega_n^p \frac{1}{p_0^2(q_j) + i\varepsilon - p_n{}^2}\right] m\mathcal{G}^{ml}_{\alpha\alpha''}(p_i p_0 q_j) \quad l \neq N_q$$

where the two smooth functions now include the appropriate interpolations.

$$\mathcal{F}^m_{\alpha\alpha''}(p_i q_j q_l) = q_l^2 \sum_{n=0}^{N_p-1}\tilde{t}_l\left(p_i, p_n; E - \frac{3q_j^2}{4m}\right)\sum_k \omega_k^x S_n(\pi(q_j q_l x_k))\ 2G_{\alpha\alpha''}(q_j q_l x_k)\ \frac{mS_m(\pi'(q_j q_l x_k))}{mE_d - \pi'(q_j q_l x_k)^2}$$

$$\mathcal{G}^{ml}_{\alpha\alpha''}(p_i p_n q_j) = p_n{}^2\ \tilde{t}_l\left(p_i, p_n; E - \frac{3q_j^2}{4m}\right)\sum_{k=0}^{N_x}\omega_k^x\ 2\tilde{G}_{\alpha\alpha''}(p_n q_j x_k)\ \frac{m\, S_m(\tilde{\pi}(p_n q_j x_k))\tilde{S}_l(\tilde{\chi}(p_n q_j x_k))}{mE_d - \tilde{\pi}(p_n q_j x_k)^2}$$

($\tilde{t}$ is also available at $p_0(q_j)$!)

This completely defines the kernel. Now we come back to the inhomogeneity

$$\sum_{\alpha''} \int dp'' p''^2 dq'' q''^2 \, \langle \, p \, q \, \alpha \, | \, \tilde{t}_{12} \, P \, | \, p'' \, q'' \, \alpha'' \rangle \langle \, p'' \, q'' \, \alpha'' \, | \, b \, \rangle = \int_{-1}^{1} dx \sum_{\alpha''} \tilde{t}_l \left(p, \pi(qq_0 x); E - \frac{3q^2}{4m} \right) \; 2G_{\alpha\alpha''}(qq_0x) \delta_{l'0} \; \varphi(\pi'(qq_0x)) \; Y_{\lambda 0}(\hat{q}_0) \; (0 \, \lambda' \, L \, , 0 \, 0 \, M \,)$$

or in discretized form

$$\mathscr{H}_\alpha(p_i q_j) = \sum_k \omega_k^x \sum_{\alpha''} \tilde{t}_l \left(p_i, \pi(q_j q_0 x_k); E - \frac{3q_j^2}{4m} \right) \; 2G_{\alpha\alpha''}(q_j q_0 x_k) \delta_{l'0} \; \sum_n S_n(\pi'(q_j q_0 x_k)) \varphi(p_n) \; Y_{\lambda 0}(\hat{q}_0) \; (0 \, \lambda' \, L \, , 0 \, 0 \, M \,)$$

The example code uses a standard library (numpy) to solve the resulting set of linear equations.

$$\sum_{ml\alpha} \left[\; \delta_{\alpha\alpha''} \delta_{im} \delta_{jl} - \mathscr{K}^{(1)}_{\alpha\alpha''}(p_i q_j, p_m q_l) - \mathscr{K}^{(2)}_{\alpha\alpha''}(p_i q_j, p_m q_l) \; \right] \; \tilde{T}_{\alpha''}(p_m q_l) = \mathscr{H}_\alpha(p_i q_j)$$

This can be solve independently for each (conserved L). However, again several L contribute to the cross sections.

For completeness, we now look at the scattering amplitude for elastic scattering (breakup could be a project!)

$$M_{b'b} = \langle\, b' \,|\, P\, (E_b - H_0)\, |\, b \rangle + \langle\, b' \,|\, P \,|\, T_{12} \,\rangle$$

The first part can be directly calculated without using a partial wave decomposition (advisable!)

$$\langle\, b' \,|\, P\, (E_b - H_0)\, |\, b \rangle = \frac{1}{4\pi} \varphi_{l=0}\left(\left| \vec{q_0} + \frac{1}{2}\vec{q_0'} \right| \right) \varphi_{l=0}\left(\left| -\vec{q_0}' - \frac{1}{2}\vec{q_0} \right| \right) \left(E_d - \frac{1}{m} \left| -\vec{q_0}' - \frac{1}{2}\vec{q_0} \right|^2 \right)$$

For elastic scattering $|\vec{q_0}| = |\vec{q_0'}| = q_0$. The vectors only depend on the scattering angle ϑ: $\vec{q_0} = \begin{pmatrix} 0 \\ 0 \\ q_0 \end{pmatrix}$ and $\vec{q_0'} = \begin{pmatrix} q_0 \sin\vartheta \\ 0 \\ q_0 \cos\vartheta \end{pmatrix}$

The second requires the treatment of the bound state pole:

$$\langle\, b' \,|\, P \,|\, T_{12} \,\rangle = \int_0^\infty dq'' \frac{\frac{4m}{3}}{q_0^2 + i\varepsilon - q''^2} \underbrace{q''^2 \sum_{\alpha\alpha''} \delta_{l0} \int dx \varphi_{l=0}\left(\pi(q_0 q'' x)\right) Y^*_{\lambda 0}(\hat{q}_0')\, (\, 0\, \lambda\, L\, , 0\, 0\, M\,)\, 2G_{\alpha\alpha''}(q_0 q'' x) \tilde{T}_{\alpha''}(\pi'(q_0 q'' x) q'')}_{I(\vartheta q_0 q'')}$$

$$= \int_0^{q_{max}} \frac{4m}{3} \frac{I(\vartheta q_0 q'') - I(\vartheta q_0 q_0)}{q_0^2 - q''^2} + \left[\ln \frac{q_{max} + q_0}{q_{max} - q_0} - i\pi \right] \frac{4m}{6q_0}\, I(\vartheta q_0 q_0)$$

Please check the implementation in the Jupyter notebook!