

Lecture 7

Part II: Integral equations for quantum mechanical few-body problems

In the previous lectures, you discussed Monte Carlo techniques mostly for the example of Ising model.

In the next weeks: **quantum mechanical two- and three-particle problems ((mostly) in momentum space).**

Dynamical equations: **integral equations** → discretization → sets of linear equations.

Linear equations **solved directly** using standard libraries or **solved iteratively** (later).

Results: exact solutions of the algebraic equations.

Discretization needs to be carefully checked to control the numerical uncertainty.

II.1 Two-body bound state problem

Quantum mechanical two-body state problem: stationary **Schrödinger equation** (non-rel., for short range interactions, no Coulomb)

$$\hat{H} |\Psi\rangle = E |\Psi\rangle$$

E<0 for the bound state (Why is this necessarily the case?)

Hamiltonian separated in kinetic energy \hat{T} and potential \hat{V} : $\hat{H} = \hat{T} + \hat{V}$

Single particle coordinates, e.g. position or momentum:

$$\vec{r}_1, \vec{r}_2 \quad \text{or} \quad \vec{k}_1, \vec{k}_2$$

Exploit translation invariance  **Jacobi coordinates**

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{p} = \frac{1}{m_1 + m_2} \left(m_2 \vec{k}_1 - m_1 \vec{k}_2 \right)$$

$$\vec{R} = \frac{1}{m_1 + m_2} (m_1 \vec{r}_1 + m_2 \vec{r}_2)$$

$$\vec{P} = \vec{k}_1 + \vec{k}_2$$

(please convince yourself that $\vec{k}_1 \vec{r}_1 + \vec{k}_2 \vec{r}_2 = \vec{p} \vec{r} + \vec{P} \vec{R}$,

also note that the Jacobian for changing variables $\vec{r}_1, \vec{r}_2 \leftrightarrow \vec{r}, \vec{R}$ and $\vec{k}_1, \vec{k}_2 \leftrightarrow \vec{p}, \vec{P}$ is one)

Express the Schrödinger equation using **Jacobi momentum eigenstates** $|\vec{p} \vec{P}\rangle$ (unity operator) $\int d^3p' d^3P' |\vec{p}' \vec{P}'\rangle \langle \vec{p}' \vec{P}'| = \mathbb{1}$

$$\left(\frac{\vec{p}^2}{2\mu_{12}} + \frac{\vec{P}^2}{2M_{12}} \right) \psi(\vec{p}, \vec{P}) + \underbrace{\int d^3p' \langle \vec{p} | \hat{V} | \vec{p}' \rangle \psi(\vec{p}', \vec{P})}_{\psi(\vec{p})\phi(\vec{P})} = E \psi(\vec{p}, \vec{P})$$

Separate off the **center of mass (CM)** motion: $\left(\bar{E} - \frac{\vec{p}^2}{2\mu_{12}} \right) \psi(\vec{p}) = \int d^3p' \langle \vec{p} | \hat{V} | \vec{p}' \rangle \psi(\vec{p}') \quad (*)$

Intrinsic energy: $\bar{E} = E - \frac{P^2}{2M_{12}}$ reduced mass: $\mu_{12} = \frac{m_1 m_2}{m_1 + m_2}$ and $M_{12} = m_1 + m_2$ (from now on: use E for the intrinsic energy)

For numerical solution: equation (*) is still **not** suitable.

- spectrum of the kinetic operator (and also Hamiltonian) is unbound.
- not interested in states with larger eigenvalues (high excitations, not the ground state and low excitations).

Equation can be easily transformed so that the **eigenvalue spectrum is bounded**:

$$\psi(\vec{p}) = \frac{1}{\bar{E} - \frac{\vec{p}^2}{2\mu_{12}}} \int d^3p' \langle \vec{p} | \hat{V} | \vec{p}' \rangle \psi(\vec{p}')$$

- Zero is only one accumulation point of the eigenvalues of this kernel.
- Equation is compact and suitable for **solution by discretization**.

Partial wave decomposition to reduce the dimensionality of the problem:

$$\langle \vec{p} | \tilde{p}lm \rangle = \frac{\delta(p - \tilde{p})}{p\tilde{p}} Y_{lm}(\hat{p}) \quad \text{or} \quad \psi(\vec{p}) = \sum_{lm} \psi_{lm}(p) Y_{lm}(\hat{p}) = \sum_{lm} \psi_l(p) Y_{lm}(\hat{p}) \quad \text{or} \quad \sum_{ml} \int d\tilde{p} \tilde{p}^2 |\tilde{p}lm\rangle \langle \tilde{p}lm| = \mathbb{1}$$

Rotational invariance 

$$V_{lm,l'm'}(p, p') = \int d\hat{p} d\hat{p}' Y_{lm}^*(\hat{p}) V(\vec{p}, \vec{p}') Y_{l'm'}(\hat{p}') = V_l(p, p') \delta_{ll'} \delta_{mm'}$$

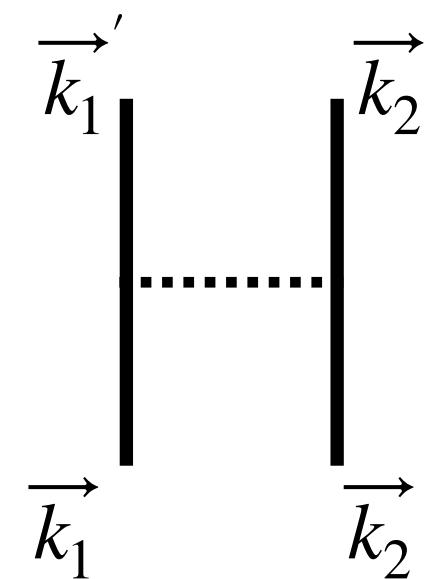
Schrödinger equation reduces to one dimensional integral equation

$$\psi_l(p) = \frac{1}{\bar{E} - \frac{p^2}{2\mu_{12}}} \int dp' p'^2 V_l(p, p') \psi_l(p')$$

Aim today: solve this equation numerically for a realistic choice for V .

Interaction

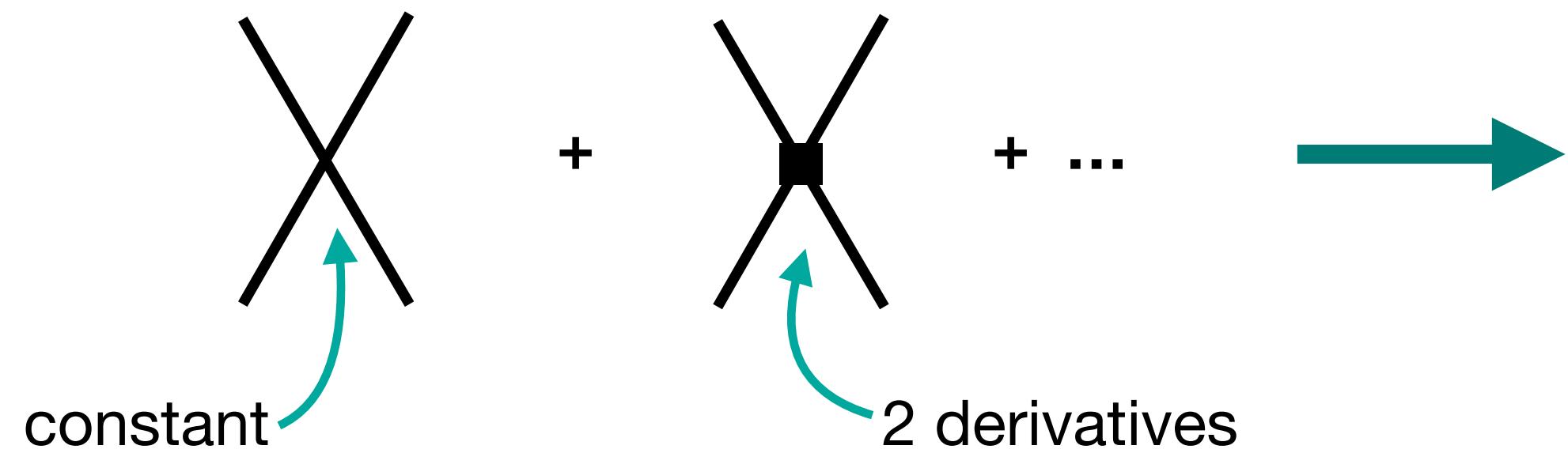
Typically, the interaction is based on some kind of **one boson exchange (OBE)** diagram, e.g.


$$\vec{k}_1' \quad \vec{k}_2' \\ \vec{k}_1 \quad \vec{k}_2$$

→ $V(\vec{p}', \vec{p}) \propto \frac{1}{\vec{q}^2 + m_B^2}$

Note that for the photon $m_B = 0$, we will not consider this case

For small momenta, $|\vec{q}| \ll m_B$, such interactions can be expanded:


$$\text{constant} + \text{2 derivatives} \rightarrow V(\vec{p}', \vec{p}) \propto C_0 + C_2 (\vec{p}^2 + \vec{p}'^2) + C'_2 \vec{p} \cdot \vec{p}' + \dots$$

Typically, a combination of these kinds of interactions insures that **long and short range physics** is included and guarantees **renormalizability**.

Caveat: both types of interactions require regularization, otherwise integrals are not well defined:

$$V(\vec{p}', \vec{p}) \longrightarrow f_\Lambda(p) V(\vec{p}', \vec{p}) f_\Lambda(p') \quad \text{or} \quad V(\vec{q}) \longrightarrow f_\Lambda(q) V(\vec{q})$$

where

$$f_\Lambda(p) = \exp\left(-\frac{p^2}{\Lambda^2}\right) \quad \text{or} \quad f_\Lambda(q) = \exp\left(-\frac{q^2 + m_B^2}{\Lambda^2}\right)$$

We will see later

- for **low energy observables**, results will **not strongly depend on the regularization** or even the kind of interaction used
- properly adjusts the short distance behavior by adding/adjusting the **short distance counter terms**.

As mentioned before: except for a few cases, even with these rather simple interactions, the problem cannot be solved analytically. Therefore, we need to solve the problem numerically.

Numerical techniques

Discretize integral using a standard quadrature formulae (below: a **modified Gauss-Legendre** quadrature)

$$\int_0^\infty dp f(p) \approx \int_0^{p_{max}} dp f(p) \approx \sum_{i=1}^N \omega_i f(p_i)$$

using N grid points p_i and weights ω_i (for such weights see for example "Numerical Recipes" Chapter 4).

Based on this grid



approximation to the Schrödinger equation (for $i, j = 1, \dots, N$)

$$\underbrace{\psi_l(p_i)}_{c_i} = \frac{1}{E - \underbrace{\frac{p_i^2}{2\mu_{12}}}_{A_{ii}}} \sum_j \omega_j p_j^2 V(p_i, p_j) \underbrace{\psi_l(p_j)}_{c_j}$$

Integral equation



homogeneous set of linear equations $c_i = A_{ij}(E) c_j$ or more generally $\lambda c_i = A_{ij}(E) c_j$.

Numerical problem: **find energy E for which the eigenvalue $\lambda = 1$ is in the spectrum of $A(E)$.**

Eigenvector \vec{c} defines the wave function at the grid points $\psi_l(p_i) = c_i$.

A few technicalities:

1. **partial wave representation of the one-boson exchange (OBE) interaction**

$$V_l(p, p') = \frac{1}{2l+1} \sum_{lm} \int d\hat{p} d\hat{p}' Y_{lm}^*(\hat{p}) Y_{lm}(\hat{p}') \frac{1}{(\vec{p} - \vec{p}')^2 + m_B^2} = 2\pi \int_{-1}^1 dx P_l(x) \frac{1}{p^2 + p'^2 - 2pp'x + m_B^2}$$

$\frac{1}{4\pi} P_l(x)$ Legendre polynomial

2. **Standard numerical libraries** (Numerical recipes, gsl, numpy, ...): **routines to define grid points and integration weights for Gauss-Legendre integration.** (in the example in the Jupyter notebook `numpy.polynomial.legendre.leggauss(nx)` is used).

By definition, these grid points are suitable for an integration interval $[-1,1]$.

For integration over an interval $[0, p_b]$, we map these grid points by

$$x \longrightarrow p(x) = \frac{1+x}{\frac{1}{p_a} - \left(\frac{1}{p_a} - \frac{2}{p_b} \right)x} \quad \text{with} \quad p'(x) = \frac{\left(\frac{2}{p_a} - \frac{2}{p_b} \right)}{\left(\frac{1}{p_a} - \left(\frac{1}{p_a} - \frac{2}{p_b} \right)x \right)^2} > 0$$

→ $\int_0^{p_b} dp f(p) = \int dx p'(x) f(p(x)) \approx \sum_{i=1}^N \underbrace{\omega_i}_{\omega_i} \underbrace{p'(x_i)}_{p_i} f(\underbrace{p(x_i)}_{p_i})$ (note that $[-1,0] \rightarrow [0, p_a]$ and $[0,1] \rightarrow [p_a, p_b]$)

Also linear transformation: $x \longrightarrow p(x) = \frac{p_b + p_c}{2} + \frac{p_c - p_b}{2}x$ (maps $[-1,1] \rightarrow [p_b, p_c]$)

3. Eigenvalue spectrum of the matrix A is bounded even when the dimensionality increases.
One accumulation point at zero.

Considering a scaled potential: **ground state corresponds to the largest (positive) eigenvalue**
first excited state to the second one, etc.

→ required are **few, largest eigenvalues and their dependence on E** for negative energies
 n -th bound state \longleftrightarrow n -th eigenvalue $\lambda(E) = 1$.

Simple numerical method to find E : **secant method**

Linear approximation, starting from two estimated solutions E_1 and E_2

→ improved approximation to the solution by

$$E = E_2 + \frac{E_1 - E_2}{\lambda(E_1) - \lambda(E_2)}(1 - \lambda(E_2))$$

The approximation can then be further improved by repeating the improvement for $E_1 = E_2$ and $E_2 = E$.

4. Approximation to the wave function $\psi_l(p_i) = c_i$ (unnormalized) in momentum space

Often it is of interest to get the wave function in **configuration space**, too.

$$\psi(\vec{r}) = \int d^3p \frac{1}{(2\pi)^{3/2}} \exp(+i\vec{p}\cdot\vec{r}) \psi(\vec{p})$$

natural units: $\hbar = c = 1$ and $\hbar c = 1 \approx 197.327 \text{ MeV fm}$

note the normalization of momentum eigenstate: $\langle \vec{p} | \vec{p}' \rangle = \delta(\vec{p} - \vec{p}')$

same name ψ in p- and r-space

Representation of the exponential in terms of spherical harmonics and **spherical Bessel functions**

$$\exp(i\vec{p}\cdot\vec{r}) = 4\pi \sum_{lm} Y_{lm}(\hat{r}) Y_{lm}^*(\hat{p}) i^l j_l(pr)$$

 **Fourier transformation** of the partial wave components

$$\psi_l(r) = i^l \sqrt{\frac{2}{\pi}} \int_0^\infty dp p^2 j_l(pr) \psi_l(p) \quad (*)$$

Assuming wave function normalization:

$$\int dp p^2 |\psi_l(p)|^2 = \int dr r^2 |\psi_l(r)|^2 = 1$$

 root means square (rms) radius $r = \sqrt{\langle r^2 \rangle}$ from expectation value $\langle r^2 \rangle = \int_0^\infty dr r^4 |\psi_l(r)|^2$

Implementation of Fourier transform uses **interpolation** of $\psi_l(p)$ to use an **increased grid for the integration** (*).

Note that Fourier transformation **does not** require complex numbers because of rescaling of wave function (parity conservation!).

Interpolation in terms of spline functions $S_n(\pi)$

Many (!) methods for interpolation.

Maybe one of the the simplest scheme: hermitian cubic splines four grid points next to the interpolated value.

1) look for nearest grid point x_i below π . This defines $x_{i-1}, x_i, x_{i+1}, x_{i+2}$

2) find cubic polynomial that reproduces the function and its numerical derivative at x_i and x_{i+1}

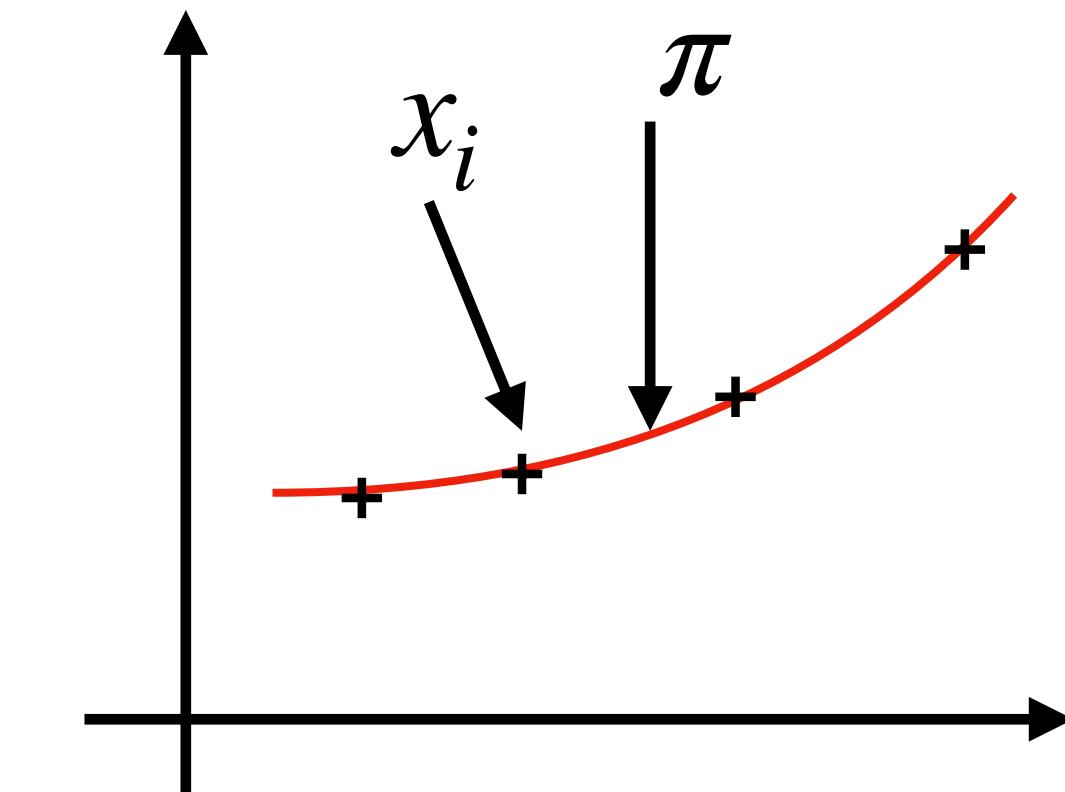
→ "cubic hermitian splines"

Nice feature: the coefficients of the polynomial are linear in the function values.

→ evaluation of the polynomials at π can be written as sum

$$f(\pi) = \sum_{i=0}^{N_p-1} S_i(\pi) f(p_i)$$

Here $S_j(\pi) = 0$ for $j \neq i-1, i, i+1, i+2$.



Close to zero a linear inter/extrapolation is useful.
At high momenta, extrapolation by zero is fine.

Notebook of the lecture gives more details and implements this interpolation (Have a look!)

The jupyter notebook coming with this lecture implements the two-body bound state problem in python.

Next weeks exercises will be dealing with the extension to a form factor calculation.

Results shown in the notebook

We start with a test of the numerical stability. Based on variations of the different grid points, we finally find that

$nx=20$, $np1=20$, $np2=10$, $pa=1$, $pb=7$ and $pc=35$

solve the problem with an accuracy better than **4 significant digits**.

parameters of the long range potential:

$m_B = 138.0$ MeV and $A = -0.15444$

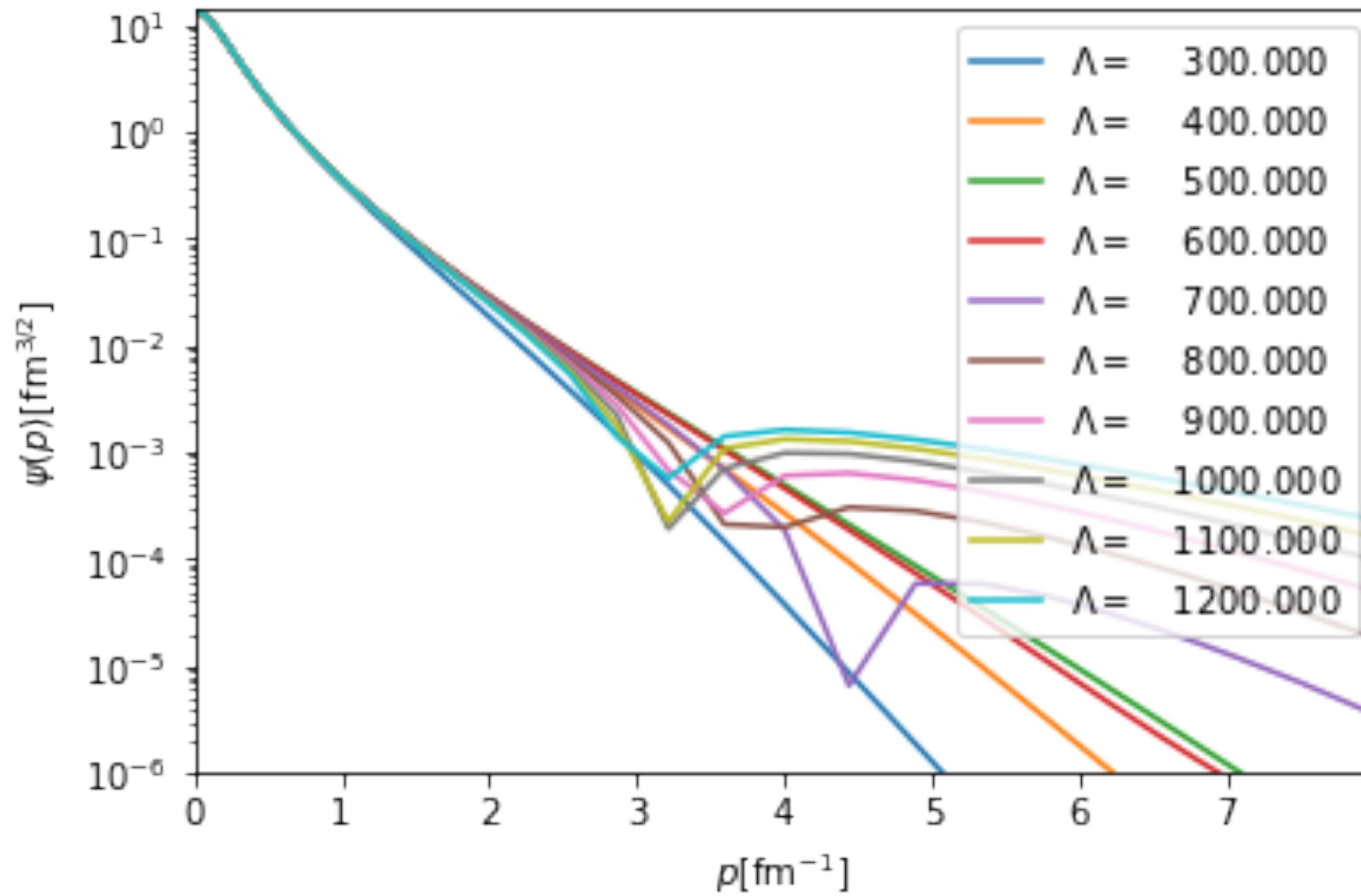
partial wave: s-wave ($l=0$)

Main result of notebook is the parameter $C_0(\Lambda)$ that leads to binding energy of -2.225 MeV!

		Fit results
Λ [MeV]	C_0 fm ²	
300.000	-9.827953E-02	
400.000	-2.820315E-02	
500.000	-4.221894E-04	
600.000	1.285743E-02	
700.000	2.016719E-02	
800.000	2.470795E-02	
900.000	2.78652E-02	
1000.000	3.030801E-02	
1100.000	3.239034E-02	
1200.000	3.431611E-02	

Solving for these parameters, results also in the wave function and allows us to perform the Fourier trafo and calculate the rms radius.

Note that the radius as defined above is the distance of the two particles. For a system of two equal mass particles, the distance to the CM of the two particles is a factor 2 smaller. In table below gives the rms radius of one particle from the CM assuming equal mass of both particles.



Energies and radii

Λ [MeV]	E [MeV]	$\sqrt{\langle r^2 \rangle / 2}$
300.000	-2.225	2.097
400.000	-2.225	2.069
500.000	-2.225	2.064
600.000	-2.225	2.065
700.000	-2.225	2.066
800.000	-2.225	2.068
900.000	-2.225	2.069
1000.000	-2.225	2.070
1100.000	-2.225	2.070
1200.000	-2.225	2.071

Lecture 8

Recap of Lecture 7

II.1 Two-body bound state problem

a) Schrödinger equation reduces to one dimensional integral equation

$$\psi_l(p) = \frac{1}{\bar{E} - \frac{p^2}{2\mu_{12}}} \int dp' p'^2 V_l(p, p') \psi_l(p')$$

b) partial wave representation of the one-boson exchange (OBE) interaction (+contact interactions)

$$V_l(p, p') = \frac{1}{2l+1} \sum_m \int d\hat{p} d\hat{p}' Y_{lm}^*(\hat{p}) Y_{lm}(\hat{p}') \frac{1}{(\vec{p} - \vec{p}')^2 + m_B^2} = 2\pi \int_{-1}^1 dx P_l(x) \frac{1}{p^2 + p'^2 - 2pp'x + m_B^2}$$

c) mapping of Gauss-Legendre grid points $[-1,1]$ to $[0, p_b]$

$$x \longrightarrow p(x) = \frac{1+x}{\frac{1}{p_a} - \left(\frac{1}{p_a} - \frac{2}{p_b} \right) x} \quad \text{with} \quad p'(x) = \frac{\left(\frac{2}{p_a} - \frac{2}{p_b} \right)}{\left(\frac{1}{p_a} - \left(\frac{1}{p_a} - \frac{2}{p_b} \right) x \right)^2} > 0$$

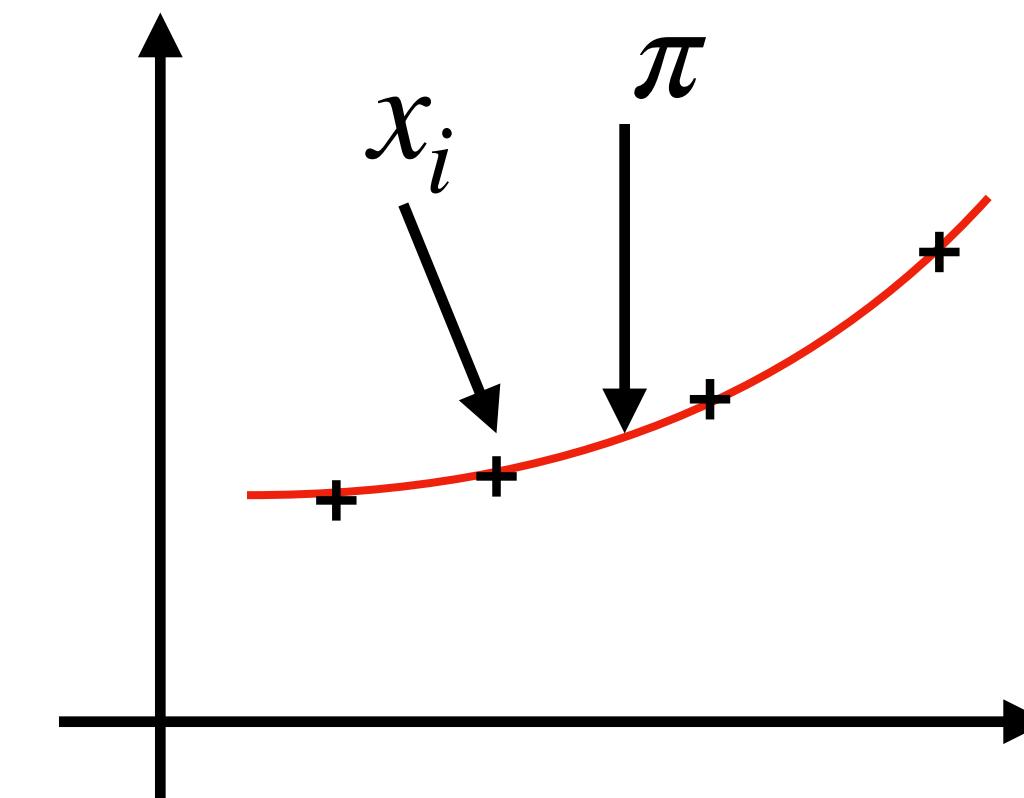
d) use secant method to improve energy in energy-dependent kernel of integral equation

given E_1 and E_2  improved approximation to the solution by $E = E_2 + \frac{E_1 - E_2}{\lambda(E_1) - \lambda(E_2)}(1 - \lambda(E_2))$

e) Fourier transformation of the partial wave components $\psi_l(r) = i^l \sqrt{\frac{2}{\pi}} \int_0^\infty dp p^2 j_l(pr) \psi_l(p)$

f) interpolation of wave functions to deviate from grid points

$$f(\pi) = \sum_{i=0}^{N_p-1} S_i(\pi) f(p_i)$$



II.2 Two-body scattering problem

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

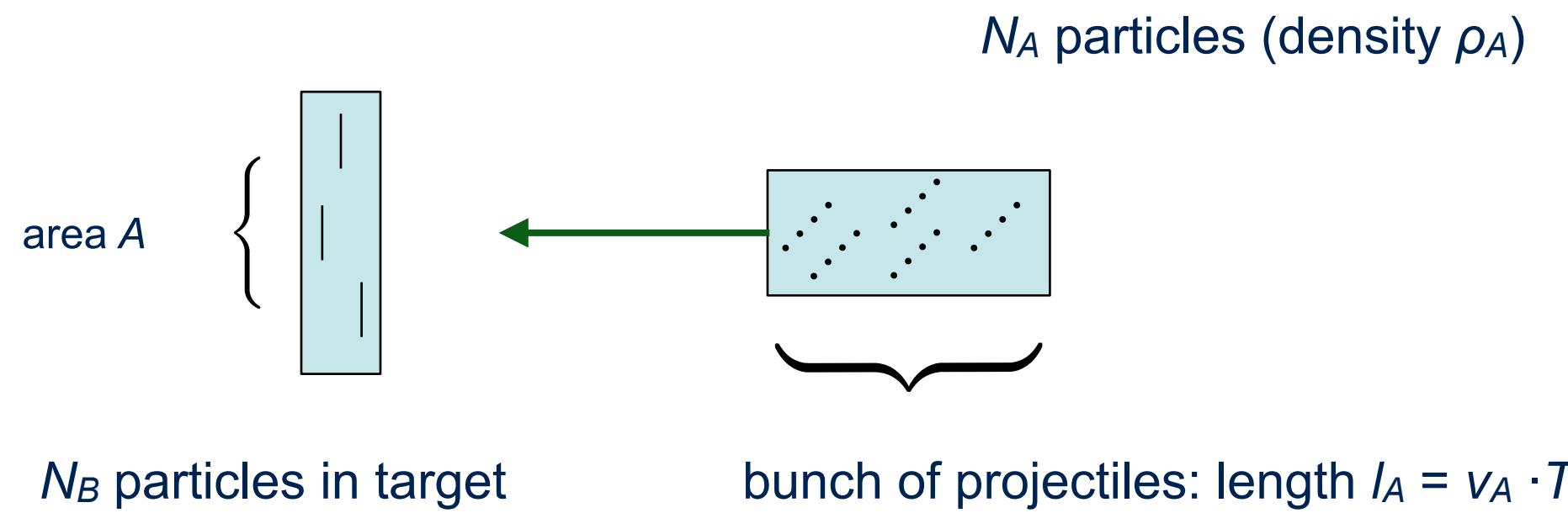
We will again use momentum space, which allows one directly include the boundary conditions into the resulting integral equation.

Technically, the main complication is the treatment of singularities of the integral equations.

The implementation of this technique will be mostly done in **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

Need to calculate the **transition probability per unit time**.

The key for this is the definition of so called "**in**" and "**out**" states.

Start at large negative times $T \rightarrow -\infty$



particles well separated from each other
time dependence given by free Hamiltonian

"initial" state 

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

Full time dependence given by full Hamiltonian:

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

The aim is to define a scattering state $|\Psi(t)\rangle$ that corresponds to $|i\rangle$ at large negative times
(use $\hat{U}_0(t)$ for time evolution operator only involving the kinetic energy).

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

This idea defines "**in**" and "**out**" states (for $T \rightarrow +\infty$):

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

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

"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

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



Problem of finding "in" and "out" states is driven by **resolvent operators**

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

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

Translation invariance the operator conserves total momentum use **relative coordinates** $S_{fi} = \langle^{(-)} | \vec{p}' | \vec{p} \rangle^{(+)}$

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

With some algebra, it is straight forward to prove the **resolvent identity**

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

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.

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


3) Introduction of the t-matrix

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

(see next slide)

S-matrix given by t-matrix



smooth function suitable for numerical calculation

t-matrix drives cross section:

$$d\sigma = (2\pi)^4 \delta(E_{p'} - E_p) \frac{1}{v_A} |t(\vec{p}', \vec{p})|^2$$

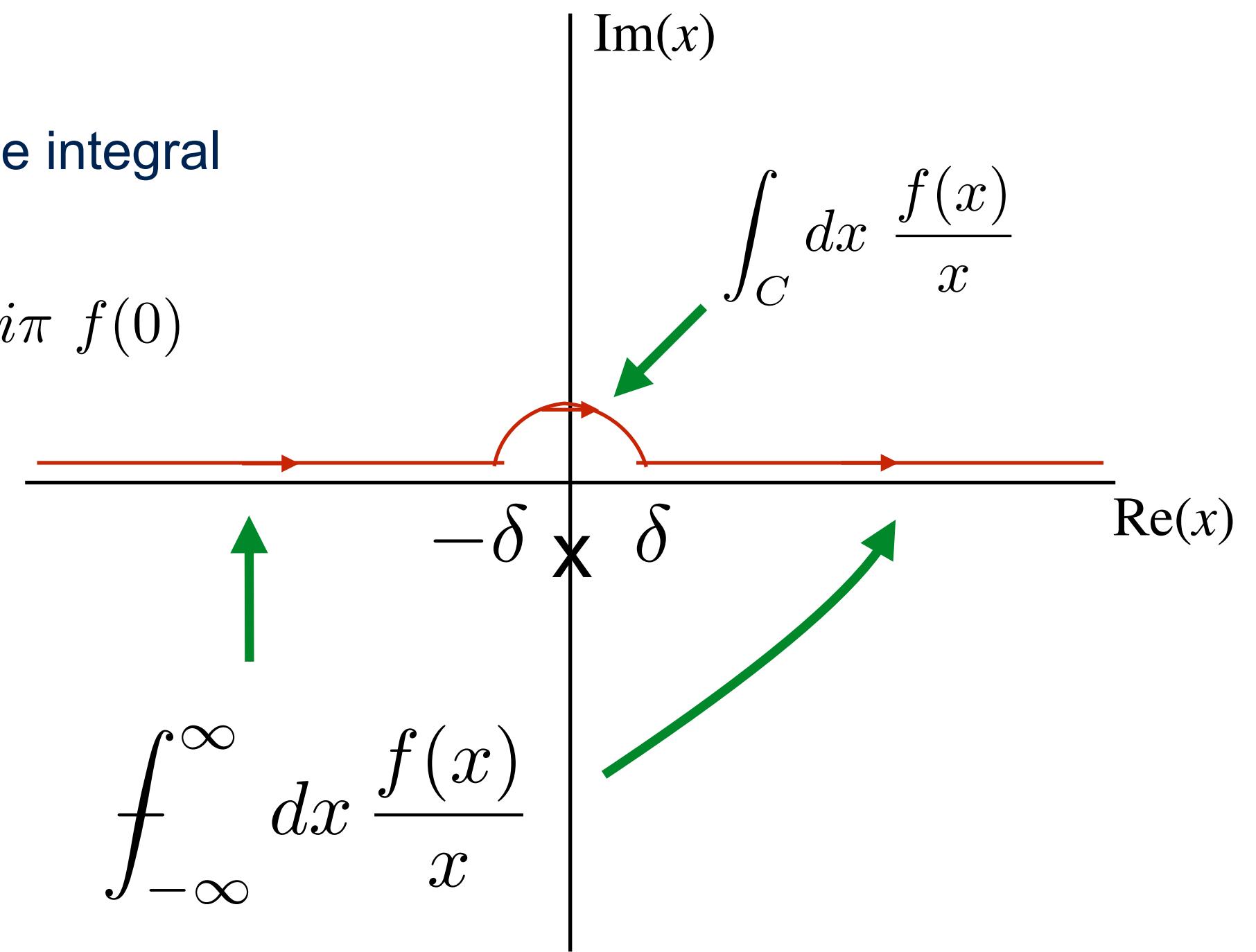
Treatment of the ε limits by integration in the complex plane

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

principal value integral

or in shorter notation

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



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

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

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

Two-body scattering observables: **on-shell t-matrix** ($E = E_{p'} = E_p$) is required.

Solution requires **half-off shell t-matrix**: $t(\vec{p}'', \vec{p})$ for $E = E_p = p^2/(2\mu)$.

Fully off-shell t-matrix ($E \neq E_p$) is important for **three-body problem**.

Expansion in terms of **partial waves**: $V(\vec{p}', \vec{p}) = \sum_{lm} Y_{lm}(\hat{p}') V_l(p', p) Y_{lm}^*(\hat{p})$  $t(\vec{p}', \vec{p}) = \sum_{lm} Y_{lm}(\hat{p}') t_l(p', p) Y_{lm}^*(\hat{p})$

Angular momentum conservation of potential directly carries over to the t-matrix.

 $t_l(p', p) = V_l(p', p) + \int_0^\infty dp'' p''^2 V_l(p', p'') \frac{1}{E_p + i\epsilon - E_{p''}} t_l(p'', p)$

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

Few side remarks on solving and checking the result

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):

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

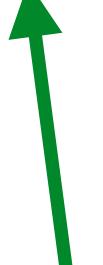
2) S-matrix is unitary

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

in a partial wave expansion

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

Unitarity implies $|S_l(p)|^2 = 1$



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

Implies representation of S- and t-matrix by a real phase shift $\delta_l(p)$:

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

Exercise 7: develop the code to obtain the t-matrix, phase shifts and cross sections

II.3 Faddeev equations for the 3-body bound state

The aim is the implementation of a **three-body bound state** problem using so-called **Faddeev equations**

Schrödinger equation:

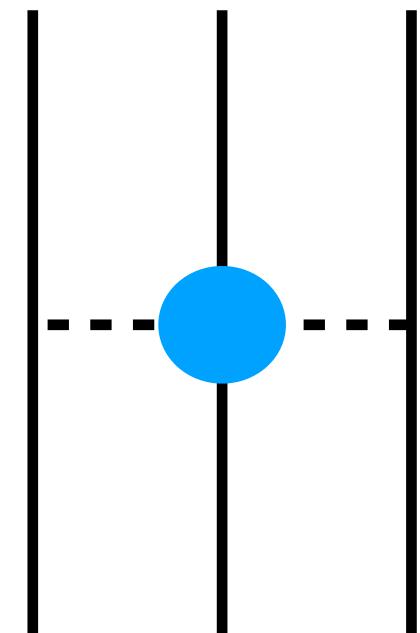
$$\hat{H} |\Psi\rangle = (\hat{H}_0 + \hat{V}_{12} + \hat{V}_{23} + \hat{V}_{31} + \hat{V}_{123}) |\Psi\rangle = E |\Psi\rangle$$

neglect three-body force

Three pair interactions V_{ij} contribute.

\hat{H}_0 is the **internal kinetic energy** (without CM motion)

\hat{V}_{123} is a possible three-body interaction (could be studied as a project later on, will be omitted here)



Here: three particles are **identical bosons**. (in exercise 7: for the cross sections particles are distinguishable (Why is this relevant?))



Enforce Pauli principle & relate the subsystems to each other!

Definition of permutation operators

Relation of Interactions using **permutation operators** P_{ij} (^ for operators is omitted now, interchange coordinates and quantum numbers)

$$H = \underbrace{T_1 + T_2 + T_3}_{H_0} + \underbrace{V_{12} + V_{23} + V_{31}}_V$$

Identity of particles: interchange coordinates relate interaction in different subsystems $V_{23} = P_{12}P_{23} V_{12} P_{23}P_{12}$

$$V_{31} = P_{13}P_{23} V_{12} P_{23}P_{13}$$

Consider single particle coordinates (momenta) to derive these relations:

$$\langle \vec{a}' \vec{b}' \vec{c}' | V_{12} | \vec{a} \vec{b} \vec{c} \rangle = \delta^{(3)}(\vec{c}' - \vec{c}) V(\vec{a}' \vec{b}', \vec{a} \vec{b})$$

Therefore, for pair (23):

\vec{V} is the same for each pair

$$\langle \vec{a}' \vec{b}' \vec{c}' | V_{23} | \vec{a} \vec{b} \vec{c} \rangle = \delta^{(3)}(\vec{a}' - \vec{a}) V(\vec{b}' \vec{c}', \vec{b} \vec{c})$$

$$\langle \vec{a}' \vec{b}' \vec{c}' | P_{12}P_{23} V_{12} P_{23}P_{12} | \vec{a} \vec{b} \vec{c} \rangle = \langle \vec{b}' \vec{a}' \vec{c}' | P_{23} V_{12} P_{23} | \vec{b} \vec{a} \vec{c} \rangle = \langle \vec{b}' \vec{c}' \vec{a}' | V_{12} | \vec{b} \vec{c} \vec{a} \rangle$$

transpositions are hermitian

$$= \delta^{(3)}(\vec{a}' - \vec{a}) V(\vec{b}' \vec{c}', \vec{b} \vec{c}) = \langle \vec{a}' \vec{b}' \vec{c}' | V_{23} | \vec{a} \vec{b} \vec{c} \rangle$$

Rewriting the Schrödinger equation

Bound state problem \rightarrow assume that $E < 0$ (even more $E < E_{2b}$)

Schrödinger equation for bound state wave function Ψ

$$(E - H_0) |\Psi\rangle = V_{12} |\Psi\rangle + P_{12}P_{23} V_{12} P_{23}P_{12} |\Psi\rangle + P_{13}P_{23} V_{12} P_{23}P_{13} |\Psi\rangle$$

$$= \left(\mathbb{I} + \underbrace{P_{12}P_{23} + P_{13}P_{23}}_{\equiv P} \right) V_{12} |\Psi\rangle$$

symmetry (Pauli principle)

abbreviation P

This allows to define a Faddeev component and relate it to the wave function:

$$|\Psi\rangle = \frac{1}{E - H_0} (\mathbb{I} + P) V_{12} |\Psi\rangle = (\mathbb{I} + P) \underbrace{\frac{1}{E - H_0} V_{12} |\Psi\rangle}_{\equiv |\psi_{12}\rangle \text{ Faddeev component}}$$

invertible since E negative

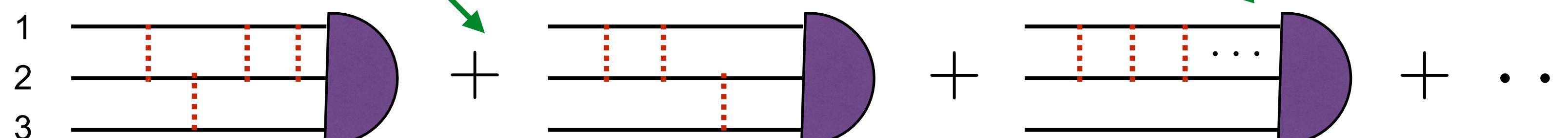
symmetric operator!

Faddeev component fulfills:

$$|\psi_{12}\rangle = \frac{1}{E - H_0} V_{12} |\Psi\rangle = \frac{1}{E - H_0} V_{12} (\mathbb{I} + P) |\psi_{12}\rangle$$

many contributions by reinserting eq.

first interaction is in (12)



one part only consists of interactions in (12)
particle 3 is not affected here

Treatment of the not-connected term

The last piece is troublesome: when in part of the operator one of the particles is not affect (unit operator in this coordinate)

- eigenvalue spectrum will have more than the accumulation point at zero
- numerical representation requires delta-function
- cannot be approximated in a finite dimensional space

Fortunately, analytical treatment is possible:

$$|\psi_{12}\rangle - \frac{1}{E - H_0} V_{12} |\psi_{12}\rangle = \frac{1}{E - H_0} V_{12} P |\psi_{12}\rangle \longrightarrow \underbrace{\left(\mathbb{I} - \frac{1}{E - H_0} V_{12} \right)}_{\text{Are we able to invert this?}} |\psi_{12}\rangle = \frac{1}{E - H_0} V_{12} P |\psi_{12}\rangle$$

yes, use **Lippmann-Schwinger equation** (see two-body scattering!)

$$\begin{aligned} \left(\mathbb{I} + \frac{1}{E - H_0} t_{12} \right) \left(\mathbb{I} - \frac{1}{E - H_0} V_{12} \right) &= \mathbb{I} - \frac{1}{E - H_0} V_{12} + \frac{1}{E - H_0} t_{12} - \frac{1}{E - H_0} t_{12} \frac{1}{E - H_0} V_{12} \\ &= \mathbb{I} - \frac{1}{E - H_0} \underbrace{\left(t_{12} - V_{12} - t_{12} \frac{1}{E - H_0} V_{12} \right)}_{0 \text{ because of LS eq.}} = \mathbb{I} \end{aligned}$$

→ **Faddeev equations**

$$|\psi_{12}\rangle = \left(\mathbb{I} + \frac{1}{E - H_0} t_{12} \right) \frac{1}{E - H_0} V_{12} P |\psi_{12}\rangle = \frac{1}{E - H_0} \left(V_{12} + t_{12} \frac{1}{E - H_0} V_{12} \right) P |\psi_{12}\rangle = \frac{1}{E - H_0} t_{12} P |\psi_{12}\rangle$$

together with the **Lippmann-Schwinger equation**

$$t_{12} = V_{12} + V_{12} \frac{1}{E - H_0} t_{12}$$

E is the binding energy and
not directly related to the two-body state
(off-shell!)

Lecture 9

Recap of Lecture 8

II.2 Two-body scattering problem

Dynamical equations can be formulated in terms of Lippmann-Schwinger equation for the t -matrix:

$$t_l(p', p) = V_l(p', p) + \int_0^\infty dp'' p''^2 V_l(p', p'') \frac{1}{E_p + i\varepsilon - E_{p''}} t_l(p'', p)$$

Relation of S-matrix, phase shifts and t -matrix $S_l(p) = \exp(2i\delta_l(p))$ and $t_l(p, p) = -\frac{\sin \delta_l(p)}{\pi \mu p} \exp(i\delta_l(p))$ with $|S_l(p)|^2 = 1$

Partial wave representation gives angular dependence

$$t(\vec{p}', \vec{p}) = \sum_{lm} Y_{lm}(\hat{p}') t_l(p', p) Y_{lm}^*(\hat{p})$$

and finally cross sections

$$d\sigma = (2\pi)^4 \delta(E_{p'} - E_p) \frac{1}{v_A} |t(\vec{p}', \vec{p})|^2$$

Form for numerical solution:

$$t_l(p', p) = V_l(p', p) + \int_0^\infty dp'' \frac{2\mu p''^2 V_l(p', p'') t_l(p'', p) - 2\mu q^2 V_l(p', q) t_l(q, p)}{q^2 - p''^2} + 2\mu q^2 V_l(p', q) t_l(q, p) \int_0^\infty dp'' \frac{1}{q^2 - p''^2} - i\pi q\mu V_l(p', q) t_l(q, p)$$

II.3 Faddeev equations for the 3-body bound state

Assume three identical bosons and define permutation operators (fermions are very similarly treated)

$$\begin{aligned} \langle \vec{a}' \vec{b}' \vec{c}' | P_{12} P_{23} V_{12} P_{23} P_{12} | \vec{a} \vec{b} \vec{c} \rangle &= \langle \vec{b}' \vec{a}' \vec{c}' | P_{23} V_{12} P_{23} | \vec{b} \vec{a} \vec{c} \rangle = \langle \vec{b}' \vec{c}' \vec{a}' | V_{12} | \vec{b} \vec{c} \vec{a} \rangle \\ &= \delta^{(3)}(\vec{a}' - \vec{a}) V(\vec{b}' \vec{c}', \vec{b} \vec{c}) = \langle \vec{a}' \vec{b}' \vec{c}' | V_{23} | \vec{a} \vec{b} \vec{c} \rangle \end{aligned}$$

Rewrite Schrödinger equation similar as in two-body case. Thereby natural separation in Faddeev components:

$$| \psi_{12} \rangle = \frac{1}{E - H_0} V_{12} | \Psi \rangle = \frac{1}{E - H_0} V_{12} (\mathbb{I} + P) | \psi_{12} \rangle$$

Disconnected and connected pieces - **Faddeev equations**

$$\begin{aligned} | \psi_{12} \rangle &= \left(\mathbb{I} + \frac{1}{E - H_0} t_{12} \right) \frac{1}{E - H_0} V_{12} P | \psi_{12} \rangle = \frac{1}{E - H_0} \left(V_{12} + t_{12} \frac{1}{E - H_0} V_{12} \right) P | \psi_{12} \rangle \\ &= \frac{1}{E - H_0} t_{12} P | \psi_{12} \rangle \end{aligned}$$

together with the **Lippmann-Schwinger equation**

$$t_{12} = V_{12} + V_{12} \frac{1}{E - H_0} t_{12}$$

E is the binding energy and
not directly related to the two-body state
(off-shell!)

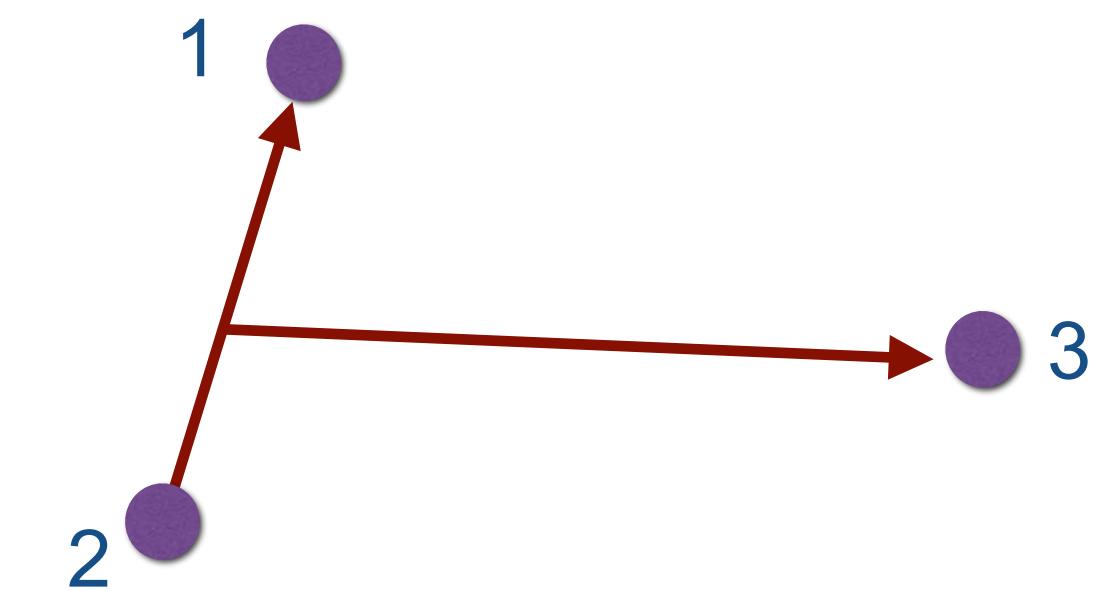
Jacobi coordinates and permutation operators

Essential new aspect of more than two-body systems

Start with single particle momenta: $\vec{k}_1 \vec{k}_2 \vec{k}_3$

Define Jacobi momenta:

$$\vec{p}_{12} = \frac{1}{2} (\vec{k}_1 - \vec{k}_2) \quad \vec{p}_3 = \frac{2}{3} \vec{k}_3 - \frac{1}{3} (\vec{k}_1 + \vec{k}_2) \quad \vec{P} = \vec{k}_1 + \vec{k}_2 + \vec{k}_3$$



or permutations (here only cyclical and anticyclical)

$$\vec{p}_{23} = \frac{1}{2} (\vec{k}_2 - \vec{k}_3) \quad \vec{p}_1 = \frac{2}{3} \vec{k}_1 - \frac{1}{3} (\vec{k}_2 + \vec{k}_3) \quad \text{and} \quad \vec{p}_{31} = \frac{1}{2} (\vec{k}_3 - \vec{k}_1) \quad \vec{p}_2 = \frac{2}{3} \vec{k}_2 - \frac{1}{3} (\vec{k}_3 + \vec{k}_1)$$

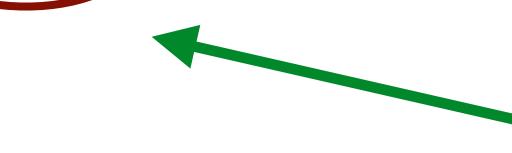
Express in terms of single particle momenta and relate with each other

$$\vec{p}_{23} = -\frac{1}{2} \vec{p}_{12} - \frac{3}{4} \vec{p}_3 \quad \vec{p}_1 = \vec{p}_{12} - \frac{1}{2} \vec{p}_3 \quad \text{and} \quad \vec{p}_{31} = -\frac{1}{2} \vec{p}_{12} + \frac{3}{4} \vec{p}_3 \quad \vec{p}_2 = -\vec{p}_{12} - \frac{1}{2} \vec{p}_3$$



matrix elements of coordinate transformations

$$(12)3 \langle \vec{p}'_{12} \vec{p}'_3 | \vec{p}_{23} \vec{p}_1 \rangle_{(23)1} = \delta^{(3)}(\vec{p}_{23} + \frac{1}{2} \vec{p}'_{12} + \frac{3}{4} \vec{p}'_3) \delta^{(3)}(\vec{p}_1 - \vec{p}'_{12} + \frac{1}{2} \vec{p}'_3)$$



Indices indicate the kind of Jacobi coordinate!
often I skip (12)3 to be shorter

Jacobi coordinates and permutation operators

Coordinate transformations  permutation operators

$${}_{(12)3}\langle \vec{p}'_{12} \vec{p}'_3 \vec{P}' | P_{12}P_{23} | \vec{p}_{12} \vec{p}_3 \vec{P} \rangle_{(12)3}$$

$$= \int d^3k_1 d^3k_2 d^3k_3 {}_{(12)3}\langle \vec{p}'_{12} \vec{p}'_3 \vec{P}' | \vec{k}_1 \vec{k}_2 \vec{k}_3 \rangle \langle \vec{k}_1 \vec{k}_2 \vec{k}_3 | P_{12}P_{23} | \vec{p}_{12} \vec{p}_3 \vec{P} \rangle_{(12)3}$$

$$= \int d^3k_1 d^3k_2 d^3k_3 {}_{(12)3}\langle \vec{p}'_{12} \vec{p}'_3 \vec{P}' | \vec{k}_1 \vec{k}_2 \vec{k}_3 \rangle \underbrace{\langle \vec{k}_2 \vec{k}_3 \vec{k}_1 | \vec{p}_{12} \vec{p}_3 \vec{P} \rangle_{(12)3}}_{= \langle \vec{k}_1 \vec{k}_2 \vec{k}_3 | \vec{p}_{12} \vec{p}_3 \vec{P} \rangle_{(23)1}} = {}_{(12)3}\langle \vec{p}'_{12} \vec{p}'_3 \vec{P}' | \vec{p}_{12} \vec{p}_3 \vec{P} \rangle_{(23)1}$$

by the change of single particle momenta,
effectively, p_{23} is set to p_{12} and p_1 to p_3

Permutation operators and coordinate transformations are equivalent!

Partial wave representation of the permutation operator

Rotation invariance — use partial wave representation

$$\langle \vec{p}_{12} | p'_{12} l'_{12} m'_{12} \rangle = \frac{\delta(p_{12} - p'_{12})}{p_{12} p'_{12}} Y_{l'_{12} m'_{12}}(\hat{p}_{12}) \quad \langle \vec{p}_3 | p'_3 l'_3 m'_3 \rangle = \frac{\delta(p_3 - p'_3)}{p_3 p'_3} Y_{l'_3 m'_3}(\hat{p}_3)$$

Conserved **total angular momentum** $\hat{\vec{L}} = \hat{\vec{l}}_{12} + \hat{\vec{l}}_3$

$$| p_{12} p_3 (l_{12} l_3) L M_L \rangle = \sum_{m_{12} m_3} (l_{12} l_3 L, m_{12} m_3 M_L) | p_{12} l_{12} m_{12} \rangle | p_3 l_3 m_3 \rangle$$

Clebsch-Gordan coefficient

Completeness relation reads

$$\mathbb{I} = \sum_{l_{12} l_3 L M_L} \int dp_{12} p_{12}^2 dp_3 p_3^2 | p_{12} p_3 (l_{12} l_3) L M_L \rangle \langle p_{12} p_3 \underbrace{(l_{12} l_3) L}_{\equiv \alpha} M_L |$$

Wanted: ${}_{(12)3} \langle p'_{12} p'_3 \alpha' M_L | p_{12} p_3 \alpha M_L \rangle_{(23)1} \leftarrow !$

Rotational invariance $\frac{1}{2L+1} \sum_{M_L} {}_{(12)3} \langle p'_{12} p'_3 \alpha' M_L | p_{12} p_3 \alpha M_L \rangle_{(23)1}$ for $L = L'$ M independence!

$$= \frac{1}{2L+1} \sum_{M_L} \int d^3 \tilde{p}'_{12} d^3 \tilde{p}'_3 d^3 \tilde{p}_{12} d^3 \tilde{p}_3 {}_{(12)3} \langle p'_{12} p'_3 \alpha' M_L | \tilde{p}'_{12} \tilde{p}'_3 \rangle_{(12)3} \quad \text{averaging removes preference for quantization axis}$$

$${}_{(12)3} \langle \tilde{p}'_{12} \tilde{p}'_3 | \tilde{p}_{12} \tilde{p}_3 \rangle_{(23)1} \quad {}_{(23)1} \langle \tilde{p}_{12} \tilde{p}_3 | p_{12} p_3 \alpha M_L \rangle_{(23)1}$$

Partial wave representation of the permutation operator

$$\frac{1}{2L+1} \sum_{M_L} {}_{(12)3} \langle p'_{12} p'_3 \alpha' M_L | p_{12} p_3 \alpha M_L \rangle {}_{(23)1}$$

$$= \frac{1}{2L+1} \sum_{M_L} \int d^3 \tilde{p}'_{12} d^3 \tilde{p}'_3 d^3 \tilde{p}_{12} d^3 \tilde{p}_3 \frac{\delta(p'_{12} - \tilde{p}'_{12})}{p'_{12} \tilde{p}'_{12}} \frac{\delta(p'_3 - \tilde{p}'_3)}{p'_3 \tilde{p}'_3} \frac{\delta(p_{12} - \tilde{p}_{12})}{p_{12} \tilde{p}_{12}} \frac{\delta(p_3 - \tilde{p}_3)}{p_3 \tilde{p}_3}$$

$$\delta^{(3)}(\vec{p}_{12} + \frac{1}{2}\vec{\tilde{p}}'_{12} + \frac{3}{4}\vec{\tilde{p}}'_3) \delta^{(3)}(\vec{p}_3 - \vec{\tilde{p}}'_{12} + \frac{1}{2}\vec{\tilde{p}}'_3) \mathcal{Y}_{l'_{12} l'_3}^{* L' M'_L}(\hat{p}'_{12} \hat{\tilde{p}}'_3) \mathcal{Y}_{l_{12} l_3}^{L M_L}(\hat{p}_{12} \hat{\tilde{p}}_3)$$

$$= \frac{1}{2L+1} \sum_{M_L} \int d\hat{p}_3 d\hat{\tilde{p}}'_3 \frac{\delta(p_{12} - \left| -\vec{\tilde{p}}'_3 - \frac{1}{2}\vec{\tilde{p}}_3 \right|)}{p_{12}^2} \frac{\delta(p'_{12} - \left| \vec{\tilde{p}}_3 + \frac{1}{2}\vec{\tilde{p}}'_3 \right|)}{p'_{12}^2}$$

$$\mathcal{Y}_{l'_{12} l'_3}^{* L' M'_L}(\vec{\tilde{p}}_3 + \frac{1}{2}\vec{\tilde{p}}'_3 \hat{\tilde{p}}'_3) \mathcal{Y}_{l_{12} l_3}^{L M_L}(-\vec{\tilde{p}}'_3 - \frac{1}{2}\vec{\tilde{p}}_3 \hat{\tilde{p}}_3)$$

$$= \int_{-1}^1 dx \frac{\delta(p_{12} - \pi_{12}(p'_3 p_3 x))}{p_{12}^2} \frac{\delta(p'_{12} - \pi'_{12}(p'_3 p_3 x))}{p'_{12}^2} \frac{1}{2L+1} \sum_{M_L} \mathcal{Y}_{l'_{12} l'_3}^{* L' M'_L}(\vec{\tilde{p}}_3 + \frac{1}{2}\vec{\tilde{p}}'_3 \hat{\tilde{p}}'_3) \mathcal{Y}_{l_{12} l_3}^{L M_L}(-\vec{\tilde{p}}'_3 - \frac{1}{2}\vec{\tilde{p}}_3 \hat{\tilde{p}}_3)$$

$$= \int_{-1}^1 dx \frac{\delta(p_{12} - \pi_{12}(p'_3 p_3 x))}{p_{12}^2} \frac{\delta(p'_{12} - \pi'_{12}(p'_3 p_3 x))}{p'_{12}^2} G_{\alpha' \alpha}(p'_3 p_3 x)$$

Using $\hat{p}'_3 = \hat{e}_z$ and \hat{p}_3 in x-z-plane

$$\int d\hat{p}_3 d\hat{\tilde{p}}'_3 \longrightarrow 4\pi 2\pi \int_{-1}^1 dx$$

$$\vec{\tilde{p}}'_3 = \begin{pmatrix} 0 \\ 0 \\ p'_3 \end{pmatrix} \quad \vec{\tilde{p}}_3 = \begin{pmatrix} p_3 \sqrt{1-x^2} \\ 0 \\ p_3 x \end{pmatrix}$$

and coupled spherical harmonics

$$\mathcal{Y}_{l_{12} l_3}^{L M_L}(\hat{p}_{12} \hat{p}_3) = \sum_{m_{12} m_3} (l_{12} l_3 L, m_{12} m_3 M_L) Y_{l_{12} m_{12}}(\hat{p}_{12}) Y_{l_3 m_3}(\hat{p}_3)$$

numerical representation of permutation!

Partial waves allowed and permutation operators

Identical bosons:

$$P_{12} |\vec{p}_{12} \vec{p}_3 \rangle = | -\vec{p}_{12} \vec{p}_3 \rangle$$

(12) transposition in PW:

$$\begin{aligned} P_{12} |p_{12} p_3 (l_{12} l_3) L M_L \rangle &= \sum_{m_{12} m_3} \int d\hat{p}_{12} d\hat{p}_3 (l_{12} l_3 L, m_{12} m_3 M_L) Y_{l_{12} m_{12}}(\hat{p}_{12}) Y_{l_3 m_3}(\hat{p}_3) P_{12} |\vec{p}_{12} \vec{p}_3 \rangle \\ &= \sum_{m_{12} m_3} \int d\hat{p}_{12} d\hat{p}_3 (l_{12} l_3 L, m_{12} m_3 M_L) (-)^{l_{12}} Y_{l_{12} m_{12}}(-\hat{p}_{12}) Y_{l_3 m_3}(\hat{p}_3) | -\vec{p}_{12} \vec{p}_3 \rangle \\ &= (-)^{l_{12}} |p_{12} p_3 (l_{12} l_3) L M_L \rangle \quad \text{excludes odd partial waves !!!} \end{aligned}$$

Permutation operators simplify

$$\begin{aligned} \langle p'_{12} p'_3 \alpha' | P_{12} P_{23} + P_{13} P_{23} | p_{12} p_3 \alpha \rangle &= \langle p'_{12} p'_3 \alpha' | P_{12} P_{23} + P_{12} P_{13} P_{23} P_{12} | p_{12} p_3 \alpha \rangle \\ &= \langle p'_{12} p'_3 \alpha' | P_{12} P_{23} + P_{12} P_{23} \underbrace{P_{12} P_{12}}_{=I} | p_{12} p_3 \alpha \rangle = 2 \langle p'_{12} p'_3 \alpha' | P_{12} P_{23} | p_{12} p_3 \alpha \rangle \end{aligned}$$

Permutation operator **conserves L** but **couples different l_{12} and l_3 !**

Partial wave representation of the Faddeev equation

Faddeev component independent of M_L $\psi_{12}^\alpha(p_{12}p_3) = \langle p_{12} p_3 \alpha | \psi_{12} \rangle$ where $\alpha = (l_{12} l_3) L$

Two-body interaction:

$$\langle p'_{12} p'_3 \alpha' | V_{12} | p_{12} p_3 \alpha \rangle = \delta_{\alpha\alpha'} \frac{\delta(p_3 - p'_3)}{p_3 p'_3} V_{l_{12}}(p'_{12}, p_{12})$$

Kinetic energy:

$$H_0 = \frac{k_1^2}{2m} + \frac{k_2^2}{2m} + \frac{k_3^2}{2m} = \frac{p_{12}^2}{2\mu_{12}} + \frac{p_3^2}{2\mu_3} + \frac{P^2}{2M} = \frac{p_{12}^2}{m} + \frac{3p_3^2}{4m} + \frac{P^2}{6m}$$
CM momentum
separates from rest

Resolvent operator (no singularity here):

$$\langle p'_{12} p'_3 \alpha' | G_0(E) | p_{12} p_3 \alpha \rangle = \delta_{\alpha\alpha'} \frac{\delta(p_{12} - p'_{12})}{p_{12} p'_{12}} \frac{\delta(p_3 - p'_3)}{p_3 p'_3} \frac{1}{E - \frac{p_{12}^2}{m} - \frac{3p_3^2}{4m}}$$

t-matrix embedded in three-body space (off-shell energies) $\langle p'_{12} p'_3 \alpha' | t_{12} | p_{12} p_3 \alpha \rangle = \delta_{\alpha\alpha'} \frac{\delta(p_3 - p'_3)}{p_3 p'_3} t_{l_{12}}(p'_{12}, p_{12}; p_3)$

The Lippmann-Schwinger equation simplifies without singularity

$$t_{12} = V_{12} + V_{12} \frac{1}{E - H_0} t_{12} \quad \longrightarrow \quad t_{l_{12}}(p'_{12}, p_{12}; p_3) = V_{l_{12}}(p'_{12}, p_{12}) + \int dp''_{12} {p''_{12}}^2 V_{l_{12}}(p'_{12}, p''_{12}) \frac{1}{\tilde{E} - \frac{{p''_{12}}^2}{m}} t_{l_{12}}(p''_{12}, p_{12}; p_3)$$

off-shell energy shifted by spectator energy: $\tilde{E} = E - \frac{3p_3^2}{4m}$

Discretized representation of the Faddeev equation

All parts together result in

$$\psi_{12}^{\alpha'}(p'_{12}p'_3) = \frac{1}{E - \frac{p'^2_{12}}{m} - \frac{3p'^2_3}{4m}} \int_{-1}^1 dx \int_0^\infty dp_3 p_3^2 t_{\alpha'}(p'_{12}\pi'_{12}(p'_3 p_3 x); p'_3) G_{\alpha'\alpha}(p'_3 p_3 x) \psi_{12}^\alpha(\pi_{12}(p'_3 p_3 x) p_3)$$

Eigenvalue equation depends on E

Needs to be varied until eigen value 1 is in the spectrum

A few notes on the discretization:

momenta need to be discretized using N_p and N_q momenta

$$\psi_{12}^\alpha(p_{12}p_3) \longrightarrow \psi(p_i q_j \alpha) \equiv \psi(i + j N_p + \alpha N_p N_q)$$

Faddeev components can be label by one common index



for the shifted momenta an interpolation is necessary (see lecture 7)

use representation as sum of function values

$$f(\pi) = \sum_{i=0}^{N_p-1} S_i(\pi) f(p_i)$$

grid points and corresponding integration weights: p_i, ω_i^p , q_j, ω_j^q and x_k, ω_k^x

This leads to the matrix equation (depending on 3-index $i, k, \alpha ..$)

$$\psi(ij\alpha) = \sum_{i'j'\alpha'} K(ij\alpha, i'j'\alpha') \psi(i'j'\alpha')$$

Discretized representation of the Faddeev equation

K can be read off

$$K(ij\alpha, i'j'\alpha') = \frac{1}{E - \frac{p_i^2}{m} - \frac{3q_j^2}{4m}} \sum_k \omega_k^x \omega_{j'}^q q_{j'}^2 \sum_m S_m(\pi'_{12}(q_j q_{j'} x_k)) t_{\alpha'}(p_i p_m; q_j) G_{\alpha\alpha'}(q_j q_{j'} x_k) S_{i'}(\pi_{12}(q_j q_{j'} x_k))$$

Note that there are no integration weights for p required (just interpolations).
Also note that the matrix equation introduces an additional sum over $i'j'\alpha'$

Example notebook

- need to discuss in open hour
- uses `numpy.linalg.solve` for the Lippmann-Schwinger equation and `np.linalg.eig` for eigenvalues
- avoids using for loops to improve performance
- physics: use previous interaction → binding energies are not very cutoff dependent
- At low momenta, partial wave decomposed amplitudes have a definite behavior as $\psi_l(p) \propto p^l$
At high orbital angular momenta, this is not well approximated by a cubic polynomial.
Therefore, the notebook uses (requires good threshold behavior of f!)

$$f_l(\pi) = \sum_n S_n(\pi) \pi^l \frac{f_l(p_n)}{p_n^l}$$

Iterative solution

Usual eigenvalue/-vector solvers scale with dimension N^3 → performance is poor even for 3-body problem

extension to 4-body problem leads to orders of magnitude larger dimension (but sparse matrices)

we only need one eigenvalue (for the ground state)

→ Iterative solution much more performant

Basic idea: interested in largest eigenvalue
spectrum of linear operator has only zero as accumulation point.

generate low dimensional basis by application of linear operator to arbitrary starting vector v_0
 $\{v_0, K v_0, K^2 v_0, K^3 v_0, \dots, K^n v_0\}$ (**Krylov subspace**)

scaling with dimension better than $\propto n N^2$ (Why better than this scaling?)

also works for homogeneous equations when v_0 is appropriately chosen

How to avoid collecting almost collinear vectors in basis?

Arnoldi-Lanczos algorithm

Usual eigenvalue/-vector solvers scale with dimension N^3 → performance is poor even for 3-body problem

Solving homogeneous equation $\Psi = K\Psi$ with arbitrary start vector v_0 with $\|v_0\| = 1$

Get new basis state using kernel (computationally demanding step): $w_{i+1} = K v_i$

Orthonormalize: $\tilde{w}_{i+1} = w_{i+1} - \sum_{k=0}^i |v_k\rangle\langle v_k| w_{i+1}\rangle$ and $v_{i+1} = \frac{\tilde{w}_{i+1}}{\|\tilde{w}_{i+1}\|}$

Low dimensional basis representation of eigen value equation:

$$c_i = \langle v_i | \Psi \rangle = \sum_k \langle v_i | K | v_k \rangle \langle v_k | \Psi \rangle = \sum_k B_{ik} c_k \quad B_{ij} = \begin{cases} 0 & \text{for } i > j + 1 \\ \sqrt{\langle v_{j+1} | \tilde{w}_{j+1} \rangle} = \|\tilde{w}_{j+1}\| & \text{for } i = j + 1 \\ \langle v_i | w_{j+1} \rangle & \text{for } i < j + 1 \end{cases}$$

- here: K is not symmetric → B is not tridiagonal
- use standard package to solve 10-20 dimensional linear set of equations
- eigenvector is obtained as linear combination of v_i

$$B = \begin{pmatrix} * & * & \dots & * \\ * & * & \dots & * \\ \vdots & \vdots & \ddots & \vdots \\ 0 & & & * \end{pmatrix}$$