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, we will consider **quantum mechanical two- and three-particle problems**.
We will (mostly) work **in momentum space.**

Therefore, our dynamical equations will be **integral equations** which, after discretization, turn into sets of linear equations.

The linear equations will be either solved directly using standard libraries for diagonalization of matrices or inverting matrices or (for three-body system) will be solved iteratively.

In both cases, the results will be exact solutions of the algebraic equations.
However, the **discretization needs to be carefully checked to control the numerical uncertainty**.

II.1 Two-body bound state problem

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

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

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

We will assume that the Hamiltonian can be separated in kinetic energy $\hat{T}$ and potential $\hat{V}$: $\hat{H} = \hat{T} + \hat{V}$

The motion of the particle can be described using single particle coordinates, e.g. position or momentum:

$$\vec{x_1}, \vec{x_2} \quad \text{or} \quad \vec{k_1}, \vec{k_2}$$

In order to exploit translation invariance, we introduce **Jacobi coordinates**

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

$$\vec{R} = \frac{1}{m_1 + m_2}\left(m_1 \vec{r}_1 + m_2 \vec{r}_2\right) \qquad \vec{P} = \vec{k}_1 + \vec{k}_2$$

(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)

Now we express the Schrödinger Gleichung using the basis of Jacobi momentum eigenstates $|\vec{p}\ \vec{P}\rangle$

and the unity operator in this basis $\int d^3p'\, d^3P'\ |\vec{p'}\vec{P'}\rangle\langle\vec{p'}\vec{P'}| = \mathbb{1}$

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

Finally, we separate off the **center of mass (CM)** motion and so that we are left with

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

The intrinsic energy is then given by $\bar{E} = E - \dfrac{P^2}{2M_{12}}$, $\mu_{12} = \dfrac{m_1 m_2}{m_1 + m_2}$ and $M_{12} = m_1 + m_2$

From now on, we only care about the intrinsic motion and use E for the intrinsic energy.

For the numerical solution, equation (*) is still not suitable. The spectrum of the potential operator (and also Hamiltonian) is unbound. Moreover, the states with larger eigenvalues correspond to the states we not interested in (high excitations, not the ground state and low excitations). But the **equation can be easily transformed so that the eigenvalue spectrum is bounded**.

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

Moreover, zero is only one accumulation point of the eigenvalues of this kernel. The equation is compact and suitable for solution by discretization.

In the next step, we use a partial wave decomposition to reduce the dimensionality of the problem. By

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

Due to rotational invariance the partial wave matrix elements of the potential are

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

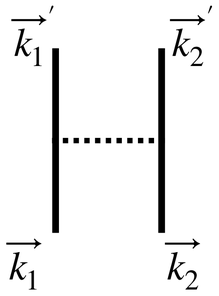
which reduces the Schrödinger equation to a one dimensional integral equation

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

It will be the aim today, to solve this equation numerically for a realistic choice for V.

Interaction

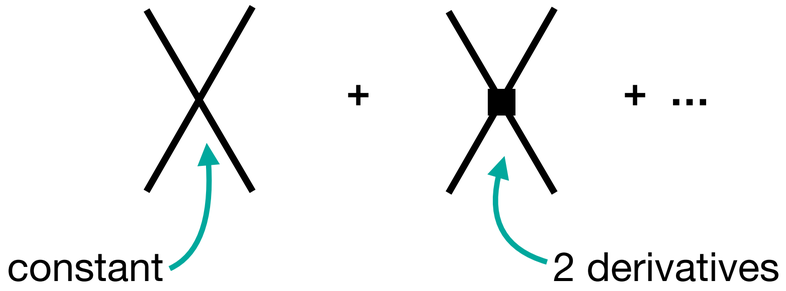
Typically, the interaction is based on some kind of **one boson exchange (OBE)** diagram, e.g.



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

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:



$$V(\vec{p}\,', \vec{p}) \propto C_0 + C_2\,(\vec{p}^{\,2} + \vec{p}^{\,\prime 2}) + C_2'\,\vec{p}\,\vec{p}\,' + \ldots$$

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 since the integrals in the Schrödinger equation will otherwise not be well defined, e.g. by

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

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 that for many **low energy observables**, results will **not strongly depend on the regularization** or even the kind of interaction used, if one 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

We discretize the integral using a standard quadrature formulae (later we will use 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, we find the following approximation to the Schrödinger equation (for $i, j = 1, \ldots, N$)

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

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

The numerical problem can now be formulated: we are interested in an energy E for which the eigenvalue $\lambda = 1$ is into the spectrum of matrix $A(E)$.

In this case, the eigenvector $\overrightarrow{c}$ defines the wave function at the grid points $\psi_l(p_i) = c_i$.

Let us prepare a few technicalities:

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

$$V_l(p,p') = \frac{1}{2l+1} \sum_m \int d\hat{p} d\hat{p}' \; Y^*_{lm}(\hat{p})\, Y_{lm}(\hat{p}') \; \frac{1}{(\vec{p} - \vec{p}\,')^2 + m_B^2}$$

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

$$= 2\pi \int_{-1}^{1} dx \; P_l(x) \; \frac{1}{p^2 + p'^2 - 2pp'x + m_B^2}$$

2. In **standard numerical libraries** (Numerical recipes, gsl, numpy, …), there are often 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

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

Using this mapping, our momentum integrals can be approximated as

$$\int_0^{p_b} dp\, f(p) = \int dx\, p'(x)\, f(p(x)) \approx \sum_{i=1}^{N} \underbrace{\omega_i p'(x_i)}_{\omega_i}\; f(\underbrace{p(x_i)}_{p_i})$$

(note that $[-1,0] \longrightarrow [0,p_a]$ and $[0,1] \longrightarrow [p_a,p_b]$)

In the example, we will also use a linear transformation

$$x \longrightarrow p(x) = \frac{p_b + p_c}{2} + \frac{p_c - p_b}{2} x$$

that maps $[-1,1] \longrightarrow [p_b,p_c]$.

3. The eigenvalue spectrum of the matrix A is bounded even when the dimensionality increases. There is one accumulation point at zero. Considering a scaled potential, one can convince oneself that the **ground state corresponds to the largest (positive) eigenvalue**. The first excited state to the second one, etc.

   Therefore, we will be interested in a **few, largest eigenvalues and their dependence on** E for negative energies. A bound state is found, if the n-th eigenvalue $\lambda(E) = 1$.

   One simple numerical method to find E is the **secant method**: Assuming a linear approximation and starting from two estimated solutions E_1 and E_2, we can find an 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. Once we have solved the eigenvalue problem using the correct binding energy, we have also found an 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.

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

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

we use the same name ψ in p- and r-space

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

Using the representation of the exponential in terms of spherical harmonics and **spherical Bessel functions**

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

one finds for the **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 that the wave function is normalized: $\int dp\, p^2 \,|\, \psi_l(p) \,|^2 = \int dr\, r^2 \,|\, \psi_l(r) \,|^2 = 1$,

the configuration space wave function can be used, e.g., to calculate the root means square (rms) radius $r = \sqrt{\langle r^2 \rangle}$ of our bound state.

$$\langle r^2 \rangle = \int_0^\infty dr\, r^4 \,|\, \psi_l(r) \,|^2$$

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

The complete Fourier transformation seems to require complex numbers due to the i^l factor.
In most cases, this can be avoided by a proper scaling of the wave function.

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 $A = -0.15444$

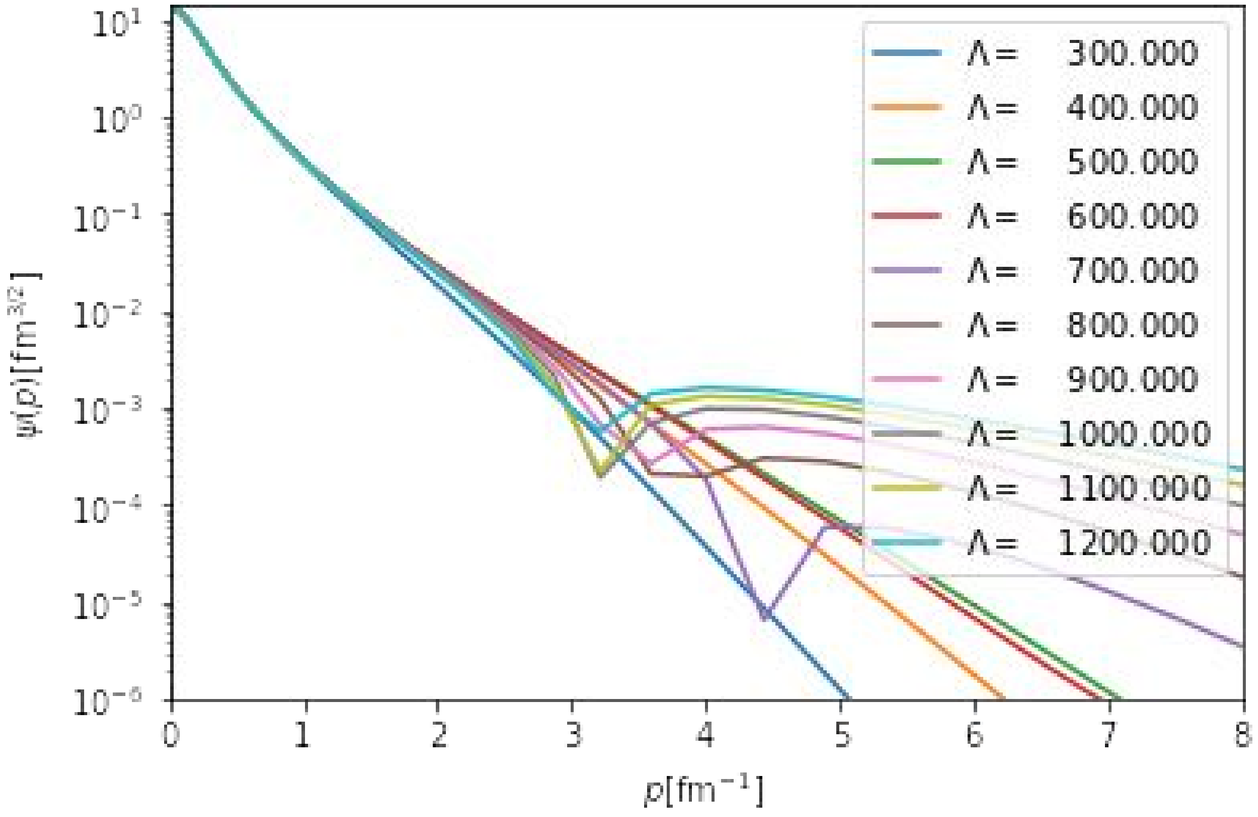
partial wave: s-wave (l=0)

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