8. Three-Body Bound-State Calculations

W. Glöckle

8.1 Motivation

The He atom, with two electrons interacting both mutually and with the nucleus, historically played a significant role in demonstrating the validity of quantum mechanics in a system more complicated than the H atom. The bound states of three nucleons, ^{3}H and ^{3}He, are still not understood, since the nuclear interactions cannot yet be calculated rigorously from an underlying theory. Therefore, tests of similar basic nature still lie in the future. At present one uses either purely phenomenological forces or forces based on meson theory [8.1] and adjusts them to describe two-nucleon observables. The question is then whether these forces are also sufficient to describe three interacting nucleons or whether in addition three-nucleon forces are needed [8.2]. Since the three-body Schrödinger equation can be solved numerically in a precise manner, the three-nucleon system plays a very significant role in answering that question. One must also investigate, in addition to the bound state, three-nucleon scattering observables [8.3] and responses to external probes [8.4].

Three-atom systems are also of great interest. Here, a very exciting phenomenon for three identical bosons is the Efimov effect [8.5], in which the number of three-body bound states increases as $\ln|a|$ if the two-body binding energy goes to zero and the scattering length $|a|$ consequently tends to infinity. Such a case is very likely realized in the ^{4}He trimer [8.6].

In the future, three-quark systems will be of interest to test quantitatively models for the nucleon or, ultimately, QCD predictions.

8.2 Three-Body Faddeev Equations

The Faddeev equations [8.7] have been proven to be very useful and we shall concentrate on them in this chapter. Other approaches used to treat three-body systems are variational calculations [8.8], the use of hyperspherical harmonics [8.9], and more recently the Green's function Monte Carlo technique [8.10].

The Faddeev equations have been discussed extensively [8.11,12]. They transcribe the content of the Schrödinger equation (including boundary conditions) in a unique manner into a set of three coupled equations, whose kernel is connected after one iteration. For the bound state, they have the form

$$\psi_1 = G_0 T_1 (\psi_2 + \psi_3) ,$$
$$\psi_2 = G_0 T_2 (\psi_3 + \psi_1) ,$$

$$\psi_3 = G_0 T_3 (\psi_1 + \psi_2) , \tag{8.1}$$

where

$$G_0 = \frac{1}{E - H_0} \tag{8.2}$$

is the free three-body propagator and T_i ($i = 1, 2, 3$) are the two-body T-operators embedded in the three-particle space. They are connected to the pair forces V_i through the Lippmann–Schwinger equation (LSE)

$$T_i = V_i + V_i G_0 T_i . \tag{8.3}$$

Here we used the convenient "odd man out" notation

$$V_i \equiv V_{jk} \qquad j \neq i \neq k . \tag{8.4}$$

The wave function is given in terms of the three Faddeev components as

$$\Psi = \psi_1 + \psi_2 + \psi_3 . \tag{8.5}$$

For identical particles the three equations (8.1) reduce to a single one owing to permutation symmetries. This is most easily seen by going back to the definition of the Faddeev components

$$\psi_i \equiv G_0 V_i \Psi . \tag{8.6}$$

Let us apply the cyclical permutation $P_{12}P_{23}$ to ψ_1:

$$\begin{aligned} P_{12}P_{23}\psi_1 &= P_{12}P_{23}G_0V_1\Psi = G_0V_2P_{12}P_{23}\Psi \\ &= G_0V_2\Psi = \psi_2 . \end{aligned} \tag{8.7}$$

Similarly

$$P_{13}P_{23}\psi_1 = \psi_3 . \tag{8.8}$$

Consequently the first equation in (8.1) reads

$$\psi_1 = G_0 T_1 (P_{12}P_{23} + P_{13}P_{23}) \psi_1 \equiv G_0 T_1 P \psi_1 \tag{8.9}$$

and the wave function is

$$\Psi = (1 + P) \psi_1 . \tag{8.10}$$

The differential form of the Faddeev equations results by using the relation

$$G_0 T_1 = \frac{1}{E - H_0 - V_1} V_1 \tag{8.11}$$

in (8.9). This leads immediately to

$$(E - H_0 - V_1) \psi_1 = V_1 P \psi_1 . \tag{8.12}$$

This form is used in configuration-space calculations [8.13], while here we use the integral form (8.9) in momentum space.

8.3 Momentum-Space Representation

The relative motion of three particles is conveniently described by Jacobi momenta

$$\begin{aligned} \boldsymbol{p}_i &\equiv \frac{1}{2}(\boldsymbol{k}_j - \boldsymbol{k}_k), \\ \boldsymbol{q}_i &\equiv \frac{2}{3}\left(\boldsymbol{k}_i - \frac{1}{2}(\boldsymbol{k}_j + \boldsymbol{k}_k)\right), \end{aligned} \tag{8.13}$$

where $(ijk) = (123), (231), (312)$. Related to them are momentum states

$$|\, \boldsymbol{p}_i \boldsymbol{q}_i\rangle \equiv |\, \boldsymbol{p}_i\rangle \otimes |\, \boldsymbol{q}_i\rangle \tag{8.14}$$

which are normalized as

$$\langle \boldsymbol{p}_i \boldsymbol{q}_i \,|\, \boldsymbol{p}_i'\, \boldsymbol{q}_i'\rangle = \delta\left(\boldsymbol{p}_i - \boldsymbol{p}_i'\right)\delta\left(\boldsymbol{q}_i - \boldsymbol{q}_i'\right) \tag{8.15}$$

and which span the space of three-body states:

$$\int \mathrm{d}\boldsymbol{p}_i \mathrm{d}\boldsymbol{q}_i \,|\, \boldsymbol{p}_i \boldsymbol{q}_i\rangle \langle \boldsymbol{p}_i \boldsymbol{q}_i \,| = 1_p \otimes 1_q \,. \tag{8.16}$$

Nuclear interactions are short-ranged and therefore act predominantly in states of low orbital angular momenta. Thus we also introduce partial-wave-projected states $|\, p\ell m_\ell\rangle$ and $|\, q\lambda m_\lambda\rangle$. Both are defined by

$$\langle \boldsymbol{k}' \,|\, k\ell m\rangle = \frac{\delta(k - k')}{kk'} Y_{\ell m}\left(\hat{k}'\right) \,. \tag{8.17}$$

It follows that

$$\langle k\ell m \,|\, k'\ell' m'\rangle = \frac{\delta(k - k')}{kk'} \delta_{\ell\ell'} \delta_{mm'} \tag{8.18}$$

and

$$\sum_{\ell m} \int \mathrm{d}k k^2 \,|\, k\ell m\rangle\langle k\ell m \,| = 1_k \,. \tag{8.19}$$

We also form states of total orbital angular momentum L:

$$|\, pq\,(\ell\lambda)\, LM\rangle = \sum_{m_\ell m_\lambda} (\ell\lambda L, m_\ell m_\lambda M) \,|\, p\ell m_\ell\rangle \,|\, q\lambda m_\lambda\rangle \,. \tag{8.20}$$

For notational simplicity we have dropped the indices that distinguish the three choices of pairs of Jacobi variables. In the following we use the convenient notation

$$|\, pq\,(\ell\lambda)\, LM\rangle_i \,, \tag{8.21}$$

which means that p and ℓ refer to the relative motion of particles j and k, while q and λ refer to the motion of particle i. The discrete set of quantum numbers $(\ell\lambda)LM$ will be abbreviated in the following by α. It is obvious that the basis states for each index obey the relations

$$\langle pq\alpha \mid p'q'\alpha' \rangle = \frac{\delta(p-p')}{pp'} \frac{\delta(q-q')}{qq'} \delta_{\alpha\alpha'} \tag{8.22}$$

and

$$\sum_{\alpha} \int \mathrm{d}pp^2 \int \mathrm{d}qq^2 \mid pq\alpha \rangle\langle\, pq\alpha \mid = 1_p \otimes 1_q \,. \tag{8.23}$$

In the following we will discuss in detail the simplest case of three identical bosons interacting by scalar pair interactions. Applications of the Faddeev equations to the dynamically richer three-nucleon system will be briefly indicated at the end of this section.

The partial-wave-projected momentum representation of a scalar pair interaction is defined by

$$\langle p\ell m \mid V \mid p'\ell'm' \rangle = \delta_{\ell\ell'} \delta_{mm'} \, v_\ell(p,p') \,. \tag{8.24}$$

This implies the representation in the three-particle basis (8.20):

$${}_1\langle pq\alpha \mid V_1 \mid p'q'\alpha' \rangle_1 = \frac{\delta(q-q')}{qq'} \delta_{\alpha\alpha'} \, v_\ell(pp') \,. \tag{8.25}$$

The operator of kinetic energy H_0 is diagonal in the Jacobi momenta

$$H_0 = \frac{p^2}{m} + \frac{3}{4m} q^2, \tag{8.26}$$

where m is the particle mass. Consequently

$$\langle pq\alpha \mid G_0(z) \mid p'q'\alpha' \rangle = \frac{\delta(p-p')}{pp'} \frac{\delta(q-q')}{qq'} \delta_{\alpha\alpha'} \frac{1}{z - \frac{p^2}{m} - \frac{3}{4m} q^2} \,. \tag{8.27}$$

The two-body T-operator in the three-particle space as given by the LSE (8.3) is clearly diagonal in the spectator quantum numbers q and λ but depends on q through the kinetic energy in G_0. The energy available to the interacting two-body subsystem is evidently $E - (3/4m)q^2$; consequently the T-operator is related to the proper two-body t-operator by

$${}_1\langle pq\alpha \mid T_1 \mid p'q'\alpha' \rangle_1 = \frac{\delta(q-q')}{qq'} \delta_{\alpha\alpha'} t_\ell \left(p, p', E - \frac{3}{4m} q^2 \right) \tag{8.28}$$

and the partial-wave-projected two-body t-operator t_ℓ for an arbitrary off-shell energy z obeys

$$\begin{aligned} t_\ell(p,p',z) &= v_\ell(p,p') \\ &+ \int_0^\infty \mathrm{d}p'' p''^2 v_\ell(p,p'') \frac{1}{z - \frac{p''^2}{m}} \, t_\ell(p'',p',z) \,. \end{aligned} \tag{8.29}$$

We thus see that the study of the three-body system requires knowledge of the two-body off-shell t-matrices.

Finally we come to the permutation operator P defined in (8.9), which connects the three different ways of grouping three particles into a pair and a single particle. The evaluation of P in the basis (8.20) is a purely geometrical problem;

$$
\begin{aligned}
&{}_1\langle pq\alpha \mid P_{12}P_{23} \mid p'q'\alpha'\rangle_1 = {}_1\langle pq\alpha \mid p'q'\alpha'\rangle_2 \\
&= \int \mathrm{d}\boldsymbol{p}''\mathrm{d}\boldsymbol{q}'' \int \mathrm{d}\boldsymbol{p}'''\mathrm{d}\boldsymbol{q}''' \; {}_1\langle pq\alpha \mid \boldsymbol{p}''\boldsymbol{q}''\rangle_1 \\
&\quad {}_1\langle \boldsymbol{p}''\boldsymbol{q}'' \mid \boldsymbol{p}'''\boldsymbol{q}'''\rangle_2 \, {}_2\langle \boldsymbol{p}'''\boldsymbol{q}''' \mid p'q'\alpha'\rangle_2 \\
&\quad = \int \mathrm{d}\hat{p} \int \mathrm{d}\hat{q} \int \mathrm{d}\hat{p}' \int \mathrm{d}\hat{q}' \; \mathcal{Y}^{LM*}_{\ell\lambda}(\hat{p}\hat{q}) \\
&\quad {}_1\langle p\hat{p}q\hat{q} \mid p'\hat{p}'q'\hat{q}'\rangle_2 \, \mathcal{Y}^{L'M'}_{\ell'\lambda'}\left(\hat{p}'\hat{q}'\right) .
\end{aligned}
\tag{8.30}
$$

$\mathcal{Y}$ describes the spherical harmonics in ℓ and λ coupled to L and M. The remaining matrix element in (8.30) is a product of two three-dimensional δ-functions, which can be chosen in different ways. We choose

$$
{}_1\langle p\hat{p}q\hat{q} \mid p'\hat{p}'q'\hat{q}'\rangle_2 = \delta\left(p\hat{p} - \tfrac{1}{2}q\hat{q} - q'\hat{q}'\right) \delta\left(p'\hat{p}' + q\hat{q} + \tfrac{1}{2}q'\hat{q}'\right) , \tag{8.31}
$$

which will be seen below to be most useful [8.14]. It follows that

$$
\begin{aligned}
{}_1\langle pq\alpha \mid p'q'\alpha'\rangle_2 &= \int \mathrm{d}\hat{q} \int \mathrm{d}\hat{q}' \frac{\delta\left(p- \mid \tfrac{1}{2}\boldsymbol{q} + \boldsymbol{q}' \mid\right)}{p^2} \\
&\times \frac{\delta\left(p'- \mid \boldsymbol{q} + \tfrac{1}{2}\boldsymbol{q}' \mid\right)}{p'^2} \mathcal{Y}^{LM*}_{\ell\lambda}\left(\widehat{\tfrac{1}{2}\boldsymbol{q} + \boldsymbol{q}'}, \hat{q}\right) \mathcal{Y}^{L'M'}_{\ell'\lambda'}\left(\widehat{-\boldsymbol{q} - \tfrac{1}{2}\boldsymbol{q}'}, \hat{q}'\right) .
\end{aligned}
\tag{8.32}
$$

After expanding the spherical harmonics the three angular integrations can be performed analytically. For a detailed discussion see, for instance, [8.12]. Here we restrict ourselves to $\ell = \lambda = \ell' = \lambda' = L = L' = 0$, which finally leads to

$$
{}_1\langle pq\alpha \mid p'q'\alpha'\rangle_2 = \tfrac{1}{2}\int_{-1}^{1} \mathrm{d}x \frac{\delta(p - \pi_1)}{p^2} \frac{\delta(p' - \pi_2)}{p'^2} \tag{8.33}
$$

with

$$
\pi_1 = \sqrt{\frac{1}{4}q^2 + q'^2 + qq'x} , \tag{8.34}
$$

$$
\pi_2 = \sqrt{q^2 + \frac{1}{4}q'^2 + qq'x} . \tag{8.35}
$$

The matrix element ${}_1\langle pq\alpha \mid P_{13}P_{23} \mid p'q'\alpha'\rangle_1$ can be reduced to the one for $P_{12}P_{23}$ by using

$$
P_{13}P_{23} = P_{23}P_{12}P_{23}P_{23} \tag{8.36}
$$

and applying P_{23} to the right and to the left. We get

$$ {}_1\langle pq\alpha \mid P_{13}P_{23} \mid p'q'\alpha'\rangle_1 = (-)^{\ell+\ell'} \, {}_1\langle pq\alpha \mid P_{12}P_{23} \mid p'q'\alpha'\rangle_1 . \tag{8.37} $$

Considering that for bosons both ℓ and ℓ' have to be even, we find that

$$ {}_1\langle pq\alpha \mid P \mid p'q'\alpha'\rangle_1 = 2 \, {}_1\langle pq\alpha \mid p'q'\alpha'\rangle_2 . \tag{8.38} $$

Now we are prepared to write down the partial-wave-projected momentum space representation of the Faddeev equation (8.9):

$$ \begin{aligned} \langle pq\alpha \mid \psi\rangle &= \langle pq\alpha \mid G_0 T P \, \psi\rangle \\ &= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \langle pq\alpha \mid TP\psi\rangle . \end{aligned} \tag{8.39} $$

We insert the completeness relation (8.23) twice and use (8.28) to obtain

$$ \begin{aligned} \langle pq\alpha \mid \psi\rangle &= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{\alpha'} \int \mathrm{d}p' p'^2 \int \mathrm{d}q' q'^2 \langle pq\alpha \mid T \mid p'q'\alpha'\rangle \\ &\times \sum_{\alpha''} \int \mathrm{d}p'' p''^2 \int \mathrm{d}q'' q''^2 \langle p'q'\alpha' \mid P \mid p''q''\alpha''\rangle \langle p''q''\alpha'' \mid \psi\rangle \\ &= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{\alpha''} \int_0^\infty \mathrm{d}p' p'^2 t_\ell \left(p, p', E - \frac{3}{4m}q^2\right) \\ &\times \int \mathrm{d}p'' p''^2 \int \mathrm{d}q'' q''^2 \langle p'q\alpha \mid P \mid p''q''\alpha''\rangle \langle p''q''\alpha'' \mid \psi\rangle . \end{aligned} \tag{8.40} $$

For the ground state, one has $L = 0$ and consequently $\ell = \lambda$. Let us consider now the simplest model case of pure s-wave interactions:

$$ v_\ell = 0 \quad \text{for} \quad \ell \neq 0. \tag{8.41} $$

Then from (8.40) it follows that only the Faddeev component

$$ \psi(pq) \equiv \langle pq\,(\ell = 0, \lambda = 0) \;\; L = 0 \;\; M = 0 \mid \; \psi\rangle \tag{8.42} $$

is nonvanishing. Using (8.33–35) and (8.38) we finally end up with

$$ \begin{aligned} \psi(pq) &= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m} \, q^2} \int_0^\infty \mathrm{d}q' q'^2 \\ &\times \int_{-1}^{1} \mathrm{d}x \; t_0 \left(p, \pi_1, E - \frac{3}{4m}q^2\right) \psi(\pi_2, q') . \end{aligned} \tag{8.43} $$

This homogenous integral equation in two variables has a nontrivial solution only at the correct binding energy E. It is for this single equation that we present numerical techniques in Sect. 8.4.

The realistic description of the three-nucleon problem is more difficult. The spins play a dynamical role. In jJ-coupling one combines the total two-body spin s with ℓ to the total two-body angular momentum j and similarily the spin 1/2 with λ to the total angular momentum J of the third particle. Then j and J are coupled to the conserved total angular momentum $\mathcal{J}$. This leads to the following basis states:

$$|\, pq\alpha\rangle \equiv |\, pq\,(\ell s)\, j\,\left(\lambda\tfrac{1}{2}\right)\; J(jJ)\; \mathcal{J}M;\left(t\tfrac{1}{2}\right) TM_T\rangle. \tag{8.44}$$

Here, we have also added isospin quantum numbers and treat the three nucleons as identical in the framework of the generalized Pauli principle.

The generalization of (8.43) then yields [8.12] the following coupled set of integral equations:

$$\begin{aligned}\langle pq\alpha \mid \psi\rangle \;=\; & \frac{1}{E-\frac{p^2}{m}-\frac{3}{4m}q^2}\sum_{\alpha'}\sum_{\alpha''}\int_0^\infty \mathrm{d}q' q'^2 \int_{-1}^{1}\mathrm{d}x \\ & \times\; \frac{t_{\alpha\alpha'}\left(p,\pi_1,E-\frac{3}{4m}q^2\right)}{\pi_1^{\ell'}}\, G_{\alpha'\alpha''}(q,q',x)\,\frac{\langle \pi_2\; q'\alpha''\;\mid \psi\rangle}{\pi_2^{\ell''}}.\end{aligned} \tag{8.45}$$

One recognizes the two-body t-matrix $t_{\alpha\alpha'}$, which allows for tensor-force couplings, and the purely geometrical functions $G_{\alpha'\alpha''}(q,q',x)$, which result from the permutation operator P. For the triton with $\mathcal{J}=1/2$ and positive parity, various numbers of discrete α-combinations, N_α, arise depending on the assumption of how many two-nucleon-force components are considered, as listed in Table 8.1. As an example for realistic three-nucleon calculations the last column shows the binding energies [8.15] based on the Argonne AV14 two-nucleon potential [8.16]. Various suggestions to explain the discrepancy with the experimental value of -8.48 MeV exist [8.17].

Table 8.1. The two-nucleon states in which V is nonvanishing together with N_α, the resulting number of discrete three-body states, and the corresponding three-nucleon binding energies.

	N_α	$E[MeV]$
${}^1S_0, {}^3S_1 - {}^3D_1$	5	-7.44
$j \le 2$	18	-7.57
$j \le 4$	34	-7.67

8.4 Numerical Methods

8.4.1 Overview

The integral equation (8.43) is easily discretized in the variable q. One introduces, for instance, a cut-off value $q_{\max}$ and distributes properly Gauss–Legendre quadrature points over the intervals $0 \le q \le q_{\max}$. However, the situation is totally different in the variable p, which under the integral takes on the skew values π_2 of (8.35). Let N_q be the number of discrete q-points and N_x the corresponding number for the x-integration, then $N_q^2 \times N_x$ π_2-values occur. Typically we will have $N_q \approx 10$ and $N_x \approx 10$, which leads to a

thousand π_2-values and therefore to too large a number of unknowns. Thus an interpolation appears to be unavoidable and adequate.

Before we discuss this point in detail, we note that the maximal value of π_2 is $3q_{\max}/2$, as is obvious from (8.35). This fact is of great importance in keeping the number of discretization points as low as possible and is a consequence of the way in which we have chosen the δ-functions in the evaluation of the permutation operator P in (8.31). The two-body subsystem is controlled by the variable p. The strong repulsive core in internucleon or interatomic forces leads to very large momentum components in the variable p, as we shall see in solving the two-body LSE. In other words the two-body t-matrix falls off very slowly. Obviously this carries over through the integral equation (8.43) to the Faddeev component $\psi(p,q)$. On the other hand the motion of the third particle is described through its distance to the center of mass of the two-body subsystem, which is the configuration-space coordinate conjugate to q. In that variable, the particle feels the two-body forces only averaged over a pair wave function, which is a less violent force. Consequently no large momentum components show up in the variable q. This will be born out in the numerical example. The value $3q_{\max}/2$ is therefore much lower than the typical cut-off value in the p-variable beyond which $\psi(p,q)$ can be neglected. Once the Faddeev equation (8.43) is solved in that smaller interval, $\psi(p,q)$ can be determined for all p-values just by quadrature using the integral equation again.

Let us now consider an interpolation in the form

$$f(x) \approx \sum_k S_k(x)\, f(x_k)\,, \tag{8.46}$$

where $S_k(x)$ are known functions and $\{x_k\}$ is a set of discrete grid points distributed over an interval in which f has to be determined. We apply this form to the p-variable in the Faddeev equation (8.43), choosing a suitable set of discrete p-points $\{p_k\}$. Then (8.43) can be approximated as

$$\begin{aligned}\psi(pq) \;&\approx\; \frac{1}{E-\frac{p^2}{m}-\frac{3}{4m}q^2} \\ &\times\; \int_0^\infty \mathrm{d}q' q'^2 \sum_{k'} \int_{-1}^{1} \mathrm{d}x\; t\left(p,\pi_1,E-\frac{3}{4m}q^2\right) S_{k'}(\pi_2)\,\psi(p_{k'},q')\,.\end{aligned} \tag{8.47}$$

Though one could afford to calculate the two-body t-matrix at all π_1-values numerically it is "cheaper" to interpolate t as well. Finally we introduce Gaussian quadrature in the variable q' and get

$$\begin{aligned}\psi(p_k,q_\ell) \;&=\; \sum_{k'}\sum_{\ell'} \left\{ \frac{1}{E-\frac{p_k^2}{m}-\frac{3}{4m}q_\ell^2}\, w_{\ell'}\, q_{\ell'}^2 \right. \\ &\times\; \left. \sum_m t\left(p_k,p_m,E-\frac{3}{4m}q_\ell^2\right) \int_{-1}^{1} \mathrm{d}x S_m(\pi_1)\, S_{k'}(\pi_2) \right\} \psi(p_{k'}\, q_{\ell'})\end{aligned} \tag{8.48}$$

with

$$\pi_1 = \sqrt{\frac{1}{4}q_\ell^2 + q_{\ell'}^2 + q_\ell q_{\ell'} x}\ ; \tag{8.49}$$

$$\pi_2 = \sqrt{q_\ell^2 + \frac{1}{4}q_{\ell'}^2 + q_\ell q_{\ell'} x}\ . \tag{8.50}$$

This is a closed set of homogeneous algebraic equations with the matrix kernel as given inside the curly brackets. The remaining x-integral will also be performed numerically by Gaussian quadrature. If N_p is the number of grid points $\{p_k\}$ for the interpolation, $N \equiv N_p \times N_q$ is the number of unknowns and the kernel is a $N \times N$ matrix.

8.4.2 Details

The Spline Interpolation

A very useful realization of the interpolation (8.46) is by cubic splines [8.18]. These are piecewise cubic polynomials defined on the intervals between the grid points x_k and joined to the adjacent intervals such that the second derivative is continuous. The spline elements $S_k(x)$ can be determined by recurrence relations, as described in detail in [8.19].

The Two-Body Potential

For a local potential $V(r)$ the momentum representation in a state of angular momentum ℓ can be found in different ways. One is to use

$$\begin{aligned}
\langle \boldsymbol{p} \mid V \mid \boldsymbol{p}' \rangle &= \frac{1}{(2\pi)^3} \int \mathrm{d}\boldsymbol{r}\ \mathrm{e}^{\mathrm{i}\left(\boldsymbol{p}-\boldsymbol{p}'\right)\cdot\boldsymbol{r}}\ V(r) \\
&= \frac{4\pi}{(2\pi)^3} \int_0^\infty \mathrm{d}r r^2 j_0\left(\mid \boldsymbol{p}-\boldsymbol{p}' \mid r\right) V(r) \\
&\equiv \tilde{V}\left(\mid \boldsymbol{p}-\boldsymbol{p}' \mid\right).
\end{aligned} \tag{8.51}$$

Then

$$\begin{aligned}
v_\ell\ (p,p') &= \langle p\ell m \mid V \mid p'\ell m \rangle = \int \mathrm{d}\boldsymbol{p}'' \int \mathrm{d}\boldsymbol{p}''' \\
&\times \langle p\ell m \mid \boldsymbol{p}'' \rangle \tilde{V}\left(\mid \boldsymbol{p}'' - \boldsymbol{p}''' \mid\right) \langle \boldsymbol{p}''' \mid p'\ell m \rangle \\
&= \int \mathrm{d}\hat{p} \int \mathrm{d}\hat{p}'\ Y_{\ell m}^*(\hat{p})\, \tilde{V}\left(\mid \boldsymbol{p}-\boldsymbol{p}' \mid\right) Y_{\ell m}\left(\hat{p}'\right).
\end{aligned} \tag{8.52}$$

Using the identity

$$\sum_m Y_{\ell m}^*(\hat{p})\, Y_{\ell m}\left(\hat{p}\,'\right) = \frac{2\ell+1}{4\pi} P_\ell\left(\hat{p}\cdot\hat{p}\,'\right) \tag{8.53}$$

we get

$$v_\ell(p,p') = 2\pi \int_{-1}^{1} \mathrm{d}x P_\ell(x)\ \tilde{V}\left(\sqrt{p^2+p'^2-2pp'x}\right). \tag{8.54}$$

A second way is to perform the transition between configuration and momentum space for a fixed ℓ:

$$\begin{aligned} v_\ell(p,p') &= \int \mathrm{d}\hat{p} Y^*_{\ell m}(\hat{p}) \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}r \mathrm{e}^{\mathrm{i}p\cdot r}\ V(r) \\ &\times \int \mathrm{d}\hat{p}\,' \frac{1}{(2\pi)^{3/2}} \mathrm{e}^{-\mathrm{i}p'\cdot r} Y_{\ell m}\left(\hat{p}\,'\right) \\ &= \frac{2}{\pi} \int_0^\infty \mathrm{d}r r^2 j_\ell(pr)\, V(r)\, j_\ell(p'r). \end{aligned} \tag{8.55}$$

In the case of a Yukawa potential

$$V(r) = V_0 \mathrm{e}^{-\mu r}/r\,, \tag{8.56}$$

which we shall use in the model calculations, both formulae (8.54) and (8.55) can be evaluated analytically with the result

$$v_\ell(p,p') = \frac{V_0}{\pi} \frac{1}{pp'} Q_\ell(z) \tag{8.57}$$

and

$$z = \frac{p^2+p'^2+\mu^2}{2pp'}. \tag{8.58}$$

Specifically for $\ell = 0$ one gets

$$v_0(p,p') = \frac{V_0}{\pi} \frac{1}{pp'} \frac{1}{2} \ln \frac{(p+p')^2+\mu^2}{(p-p')^2+\mu^2} \tag{8.59}$$

The Two-Body t-Matrix

The potential $v_\ell(p,p')$ enters into the driving term and the kernel of the LSE (8.29) for t_ℓ. The p''-integral in (8.29) can be conveniently discretized by N_p Gaussian quadrature points and we get in obvious notation

$$\begin{aligned} t_\ell(p_k,p',z) &= v_\ell(p_k,p') \\ &+ \sum_{k'} w_{k'} p_{k'}^{\prime 2} v_\ell(p_k,p_{k'}) \frac{1}{z-p_{k'}^{\prime 2}/m}\ t_\ell(p_{k'},p',z). \end{aligned} \tag{8.60}$$

For each p' and energy z this is a closed set of inhomogeneous algebraic equations with a matrix kernel of dimension $N_p \times N_p$. For a three-body bound state the two-body energies are

$$z = E - \frac{3}{4m} q^2 < 0, \tag{8.61}$$

and therefore the denominating part in (8.60) is nonsingular.

The Three-Body Eigenvalue Problem

The homogeneous Faddeev equation (8.43) can be regarded as an eigenvalue problem

$$\eta_\mu \psi_\mu \;=\; K\psi_\mu \tag{8.62}$$

with $\eta_\mu = 1$. Since the square of the Faddeev kernel is connected and therefore has a discrete spectrum, the same applies to K. The point of accumulation of the set $\{\eta_\mu\}$ is zero. Consequently there is an eigenvalue $\eta_{\max}$, which is largest in magnitude. A simple way to find $\eta_{\max}$ is the simple vector iteration method [8.18], which was popularized in the context of three-body Faddeev equations by Malfliet and Tjon [8.20]. Choosing an arbitrary state ϕ one generates

$$\phi_n \;\equiv\; K^n\phi\,, \qquad n>0, \tag{8.63}$$

and forms the ratios

$$R_n \;=\; \phi_{n+1}/\phi_n. \tag{8.64}$$

Decomposing ϕ into the set of eigenstates ψ_μ we clearly see that

$$\lim_{n\to\infty} R_n \;=\; \eta_{\max} \tag{8.65}$$

and that ϕ_n tends towards the corresponding eigenstate.

For a purely attractive interaction all the eigenvalues η_μ are positive. If E is the ground-state energy, then $\eta_{\max}$ is the physical eigenvalue 1. This can easily be seen. Assume that $\eta_{\max} > 1$; then the kernel $K/\eta_{\max}$ with a weaker two-body t-matrix $t/\eta_{\max}$ would have a bound state at the energy E contrary to the assumption that E is the lowest energy related to t.

If V has attractive and repulsive parts, negative eigenvalues will also occur and it may be that $\eta_{\max} < -1$. Then the Malfliet–Tjon (MT) method converges towards that unphysical eigenvalue. A simple algorithm to overcome this problem is given in [8.14]. First one determines $\eta_{\max}$ by the MT method. An approximate value $\eta_{\max}^{\text{appr}}$ is sufficient. Then we define

$$\phi' = (K - \eta_{\max}^{\text{appr}})\,\phi. \tag{8.66}$$

Decomposing ϕ into the set of eigenstates ψ_μ, one sees that the coefficient of the eigenstate belonging to $\eta_{\max}$ is proportinal to $(\eta_{\max} - \eta_{\max}^{\text{appr}})$. If necessary, the step from ϕ to ϕ' can be repeated in order to suppress the component belonging to $\eta_{\max}$ even more. The MT method applied to ϕ' will converge towards the eigenvalue which comes next in magnitude.

An even simpler algorithm is to replace the eigenvalue problem (8.62) by

$$(K - \eta_{\max}^{\text{appr}})\,\psi_\mu \;=\; (\eta_\mu - \eta_{\max}^{\text{appr}})\;\psi_\mu\,. \tag{8.67}$$

Then $\eta_{\max}$ is mapped onto approximately zero and the physical eigenvalue 1 onto $(1-\eta_{\max}^{\text{appr}})$, which is the largest one in magnitude. Then the MT method can be directly applied to (8.67).

In the numerical examples given below, these modifications turn out to be unnecessary. Since the energy eigenvalue E is not known, one starts with an estimated energy and determines the corresponding physical eigenvalue η. Then the energy E is varied such that $\eta(E)$ approaches the value 1. This is a simple routine searching for the zero of

$$\eta(E) - 1 \;=\; 0. \tag{8.68}$$

8.5 Model Calculations

We choose a model of three nucleons interacting via a pure s-wave potential. The interaction is averaged over singlet and triplet states and has been given in [8.20]. It is of the form

$$V(r) \;=\; -V_A \frac{\mathrm{e}^{-\mu_A r}}{r} + V_R \frac{e^{-\mu_R r}}{r}. \tag{8.69}$$

The parameters are displayed in Table 8.2 together with the two-body binding energy ϵ.

Table 8.2. The potential parameters of (8.69) and the two-body binding energy.

V_A [MeVfm]	V_R [MeVfm]	μ_A [fm^{-1}]	μ_R [fm^{-1}]	ε [MeV]
570.316	1438.4812	1.55	3.11	−0.35

In the three-body ground state of our model the space part is totally symmetric under exchange of two particles and the antisymmetric spin–isospin part of the wave function can be factored out. Therefore one has effectively the case of three identical bosons. The momentum-space potentials $v_0(p,p')$ have the form (8.59).

For the solution of the two-body LSE (8.60) we use Gaussian–Legendre quadrature points $\{p_k\}$ of the following type

$$p \;=\; \frac{(2ac-ab-bc)(1+x)+2a(b-c)}{(a-2b+c)\,x \;+\; a-c} \qquad (-1 \le x \le 1). \tag{8.70}$$

Half of the n quadrature points lies in the p-interval $(a,\ b)$ and the other half between b and c. The weights $\{w_k\}$ can be read off from

$$\mathrm{d}p \;=\; \frac{2(b-c)(a-c)(b-a)}{((a-2b+c)\,x \;+\; a-c)^2}\,\mathrm{d}x. \tag{8.71}$$

The total p-interval necessary for solving (8.60) is split into a first part, $[0, p_{\max}]$, which enters in solving the Faddeev equation (8.48), and a remaining part $[p_{\max}, p_{\text{cut}}]$. Here $p_{\max} = 3/2\ q_{\max}$ (in fact we add a small quantity to $3/2\ q_{\max}$ in order to allow for a safe interpolation) and p_{cut} is the cut-off value for the p''-integral in (8.29).

We choose the same distribution for the N_q q-points, where now $a = 0$ and $c = q_{\max}$. For a given starting energy E the LSE (8.60) is to be solved at the N_q energies $z_k = E - 3q_k^2/4m$.

It is convenient to choose the set of grid points for the spline interpolation to be identical to the quadrature points in the first p-interval. Therefore the p'-values in (8.60) are identified with that first group of points. Let that number of points be N_p. Then for each energy z the inhomogeneous set (8.60) has N_p different driving terms:

$$\sum_{k''} \left(\delta_{kk''} - \frac{w_{k''} p_{k''}^2}{z - p_{k''}^2/m} v_0(p_k, p_{k''}) \right) t(p_{k''}, p_{k'}, z) = v_0(p_k, p_{k'}) . \qquad (8.72)$$

This is a standard algebraic problem and is solved by the routine F04AEF of the NAG library.

The spline elements $S_k(p)$ are generated in two steps. A first subroutine (SPREP) prepares coefficients, which requires only the knowledge of the set of grid points $\{p_k\}$. A second subroutine (SELEM) calculates the N_p spline elements $S_k(p)$ for a given p-value.

Now we are ready to build up the Faddeev kernel in (8.48). Depending on the storage available the matrix kernel can be calculated once or built up out of prepared parts at each iteration within the MT method. We choose the second option. The structure of the kernel in (8.48) is very transparent and can be recovered easily in the code.

In Table 8.3 we display a set of "safe" discretization parameters. Here N_p^{tot} is the total number of Gaussian-quadrature p-points used for solving (8.72) out of which only the first N_p p-points are needed for solving (8.48). For the spline interpolation it is convenient to include $p = 0$ as the first point.

Table 8.3. Discretization parameters for (8.48) and (8.72).

N_p	$p_{\max}$	p_{cut}	N_p^{tot}	N_q	$q_{\max}$	N_x
19	6.3	50.0	39	10	4.0	10

The ratios R_n of (8.64) depend on p and q for small n and will become independent of these variables only for asymptotic values of n. Starting with the initial state $\phi(pq) \equiv 1$ we show in Table 8.4 the ratios R_n for the fixed p and q values $p = 0.4592\ \text{fm}^{-1}$, $q = 0.7922\ \text{fm}^{-1}$, and the maximal

Table 8.4. The minimal and maximal ratios $R_n^{(\pm)}$ of (8.64) together with the ratio $\bar{R}_n$ at the fixed values $p = 0.4592$ fm $^{-1}$, $q = 0.7922$ fm^{-1} as a function of n. The initial state is $\phi \equiv 1$.

n	$R_n{}^{(-)}$	$\bar{R}_n$	$R_n{}^{(+)}$
2	−0.422859E+01	0.552505E+00	0.165611E+01
3	−0.340999E+01	0.114284E+01	0.416641E+02
4	−0.146104E+03	0.933817E+00	0.248889E+02
5	−0.148619E+02	0.103320E+01	0.222942E+02
6	−0.485679E+01	0.998753E+00	0.292972E+01
7	−0.389955E+01	0.101066E+01	0.169167E+03
8	−0.377271E+02	0.100626E+01	0.290163E+03
9	−0.473449E+02	0.100782E+01	0.321938E+02
10	−0.592942E+00	0.100726E+01	0.652134E+01
11	0.324155E−01	0.100746E+01	0.133087E+01
12	0.919647E+00	0.100739E+01	0.118705E+02
13	0.677033E+00	0.100741E+01	0.104186E+01
14	0.995467E+00	0.100740E+01	0.118361E+01
15	0.953650E+00	0.100741E+01	0.101174E+01
16	0.100586E+01	0.100741E+01	0.102776E+01
17	0.100026E+01	0.100741E+01	0.100796E+01
18	0.100721E+01	0.100741E+01	0.100999E+01
19	0.100648E+01	0.100741E+01	0.100748E+01

deviations $R_n^{(\pm)}$ in both directions by going through all p- and q-values. The energy is $E = -7.4$ MeV. We see that a sufficiently perfect independence of p and q has not yet been reached within 19 iterations. The situation improves considerably if at a second energy the initial state ϕ is chosen to be the final one of the iteration procedure at the first energy. This is illustrated in Table 8.5. Table 8.6 demonstrates the energy search.

Including the tests with respect to variations of the discretization parameters we end up with a binding energy of $E = -7.54$ MeV.

Having reached the asymptotic value of R_n we have also found the unnormalized Faddeev component

$$\phi_n(p,q) \overset{n\to\infty}{\longrightarrow} \psi(p,q). \tag{8.73}$$

According to (8.10) the total wave function is given by

$$\begin{aligned} \Psi(\boldsymbol{p},\boldsymbol{q}) &= \frac{1}{4\pi}\Big(\psi(p,q) + \psi\Big(\Big|\frac{1}{2}\boldsymbol{p} + \frac{3}{4}\boldsymbol{q}\Big|, \Big|\boldsymbol{p} - \tfrac{1}{2}\boldsymbol{q}\Big|\Big) \\ &+ \psi\Big(\Big|\frac{1}{2}\boldsymbol{p} - \frac{3}{4}\boldsymbol{q}\Big|, \Big|\boldsymbol{p} + \frac{1}{2}\boldsymbol{q}\Big|\Big)\Big). \end{aligned} \tag{8.74}$$

Table 8.5. Same as in Table 8.4, but for the energy −7.5 MeV and using a starting vector from the end of the previous iteration at $E = -7.4$ MeV.

n	$R_n^{(-)}$	$\bar{R}_n$	$R_n^{(+)}$
2	0.998718	1.00313	1.02435
3	1.00005	1.00223	1.03643
4	1.00149	1.00212	1.00357
5	1.00181	1.00209	1.00588
6	1.00184	1.00208	1.00221
7	1.00205	1.00208	1.00250
8	1.00202	1.00208	1.00209
9	1.00207	1.00208	1.00212
10	1.00207	1.00208	1.00208

Table 8.6. Illustration of the energy search. The physical eigenvalue $\eta(E)$ of (8.62) as a function of E.

E [MeV]	$\eta(E)$
−7.4	1.0074
−7.5	1.0021
−7.6	0.99683
−7.5396	0.99999
−7.5394	1.0000

We have used the linear connection between the different sets of Jacobi momenta

$$\begin{aligned} \boldsymbol{p}_2 &= -\tfrac{1}{2}\boldsymbol{p}_1 - \tfrac{3}{4}\boldsymbol{q}_1 \,, & \boldsymbol{p}_3 &= -\tfrac{1}{2}\boldsymbol{p}_1 + \tfrac{3}{4}\boldsymbol{q}_1 \,, \\ \boldsymbol{q}_2 &= \boldsymbol{p}_1 - \tfrac{1}{2}\boldsymbol{q}_1 \,, & \boldsymbol{q}_3 &= -\boldsymbol{p}_1 - \tfrac{1}{2}\boldsymbol{q}_1 \quad . \end{aligned} \tag{8.75}$$

The state under consideration has $L = 0$ and thus depends only on p, q, and $x \equiv \hat{p} \cdot \hat{q}$. As mentioned in Sect. 8.4.1 the Faddeev component $\psi(p, q)$ leaks out in p much further than $3/2\ q_{\max}$, up to which it has been determined. We can evaluate $\psi(p, q)$ for $p > 3q_{\max}/2$ using the Faddeev equation (8.43) again; the kernel has to be built up choosing the desired p-values in the two-body t-matrix.

The two permuted Faddeev components for Ψ can be expanded into Legendre polynomials:

$$\Psi(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{4\pi} \sum_{\ell} \psi_\ell(p, q)\, P_\ell(x)\, (2\ell + 1) \tag{8.76}$$

with

$$\psi_\ell(p,q) = \int_{-1}^{1} \mathrm{d}x P_\ell(x)\,\psi\left(\sqrt{\frac{1}{4}p^2+\frac{9}{16}q^2+\frac{3}{4}pqx}, \sqrt{p^2+\frac{1}{4}q^2-pqx}\right) + \delta_{\ell 0}\psi(p,q)\,. \tag{8.77}$$

The evaluation of the x-integral requires ψ at skew values, which can be easily interpolated in terms of $\psi(p_k, q_\ell)$ using the given spline routine. Finally the normalization condition is

$$\int \mathrm{d}\boldsymbol{p} \int \mathrm{d}\boldsymbol{q}\; \Psi^2(\boldsymbol{p},\boldsymbol{q}) = \sum_\ell (2\ell+1) \int \mathrm{d}p p^2 \int \mathrm{d}q q^2\; \psi_\ell^2(p,q) = 1\,. \tag{8.78}$$

One can also normalize Ψ directly without introducing the partial wave decomposition:

$$\begin{aligned}\langle \Psi \mid \Psi \rangle &= \langle (1+P)\psi \mid (1+P)\psi \rangle \frac{1}{(4\pi)^2} \\ &= \frac{3}{(4\pi)^2}\langle \psi \mid (1+P)\psi \rangle = 3\left[\int \mathrm{d}p p^2 \int \mathrm{d}q q^2 \psi^2(pq)\right. \\ &+ 2\int \mathrm{d}p p^2 \int \mathrm{d}q q^2 \int_{-1}^{1} \mathrm{d}x \psi(pq) \\ &\times \left.\psi\left(\sqrt{\frac{1}{4}p^2+\frac{9}{16}q^2+\frac{3}{4}pqx}, \sqrt{p^2+\frac{1}{4}q^2-pqx}\right)\right] = 1.\end{aligned} \tag{8.79}$$

We leave the construction of the normalized wave function to the reader.

8.6 Exercises

The number of the various discretization points should be modified in order to get a feeling for the numerical stability.

Building up the Faddeev kernel only once for each energy instead of reconstructing it at each iteration will decrease the CPU time by about a factor of 3. Even more can be gained by vectorization.

The nucleon–nucleon interaction used has an attractive as well as a repulsive part. A similar interaction is the Malfliet–Tjon potential III (see Ref [8.20]) which gives a deuteron binding energy of -2.23 MeV. What would be the corresponding three-nucleon binding energy? The Malfliet–Tjon potential IV is purely attractive with the same deuteron binding of -2.23 MeV. Using this potential one will experience a dramatic increase in the three-nucleon binding energy, demonstrating the importance of the repulsion.

The total wave function is necessary, for instance, for the evaluation of the momentum distribution in the three-nucleon bound state. The normalized wave function can be obtained easily following the description given at the end of Sect. 8.5.

8.7 Technical Note

The following is a brief description of the NAG subroutines which are called by the program. The program `D01BCF` returns the weights and abscissae for a Gaussian quadrature, while subroutine `F04AEF` solves the algebraic equations (8.72). A more detailed description of these programs is found in the *NAG FORTRAN Library Manual.*

F04AEF

Purpose:		Calculates the solution of a set of real linear equations with multiple right-hand sides, AX=B, by Crout's factorization method.
Usage:		`CALL F04AEF (A,IA,B,IB,N,M,C,IC,WK,AA,IAA, BB,IBB,IFAIL)`
Arguments:		
A	–	real array of dimension (IA,p), where p $\geq$ N; A contains the element of the real matrix (input)
IA	–	first dimension of array A, IA $\geq$ N (input)
B	–	real array of dimension (IB,q), where q $\geq$ M; B contains the elements of the M right-hand sides (input)
IB	–	first dimension of array B, IB $\geq$ N (input)
N	–	specifies the order of matrix A (input)
M	–	specifies the number of right-hand sides (input)
C	–	real array of dimension (IC,r), where r $\geq$ M; C contains the M solution vectors (output)
IB	–	first dimension of array C, IC $\geq$ N (input)
WK	–	workspace array of dimension at least N
AA	–	real array of dimension (IAA,s) where s $\geq$ N; AA contains the Crout factorization (output)
IAA	–	first dimension of array AA, IAA $\geq$ N (input)
BB	–	real array of dimension (IBB,t) where t $\geq$ M; MM contains the M residual vectors (output)
IBB	–	first dimension of array BB, IBB $\geq$ N (input).
IFAIL	–	error indicator; before entry IFAIL must be assigned a value (IFAIL=0) (input).

D01BCF

Purpose:		Returns the weights and abscissae for a Gaussian quadrature rule with a specified number of abscissae.
Usage:		`CALL D01BCF (IT,A,B,C,D,N,WEIGHT,ABSCIS,IFAIL)`
Arguments:		
IT	–	specifies the rule type, which is Gauss–Legendre (IT=0) in the present case (input)
A	–	lower integral boundary (input)
B	–	upper integral boundary (input)
C	–	not needed presently (C=0) (input)
D	–	not needed presently (D=0) (input)
N	–	specifies the number of weights and abscissae to be returned (input)
WEIGHT	–	array of dimension N containing the N weights (output)
ABSCIS	–	array of dimension N containing the N abscissae (output)
IFAIL	–	error indicator; before entry IFAIL must be assigned a value (IFAIL=0) (input)

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