DIPLOMARBEIT

A Faddeev based R-matrix method

Ausgeführt am

Atominstitut

der Technischen Universität Wien

unter der Anleitung von

Univ.Prof. Dipl.-Ing. Dr.techn. Helmut Leeb

durch

Benedikt Raab, BSc
Böhmstraße 384, A-3970 Weitra
Matrikelnummer: 1027403

Wien, den 09.10.2017 ....
Unterschrift

Meinen Eltern

Contents

1 Introduction

Nuclear reaction theory is well developed for two-body channels. With increasing energy of the incident particle three-body exit-channels will occur. Especially for light nuclei these break-up reactions are of importance e.g. ^{17}O(n,2n)^{16}O and ^{9}Be(α,np)^{11}B which occur in nuclear fusion reaction. Such three-body exit-channels can be described within the statistical model in the unresolved resonance regime. However, this model cannot be used for three-body reactions in the resonance regime, which occur at collisions with light nuclei. In the absence of a quantitative many-body theory of light nuclear reaction systems, the R-matrix theory [1] is usually applied in the resonance regime. The R-matrix, originally introduced by Eisenbud and Wigner [1] provides an elegant description of resonances without detailed information about the internal structure of the collision partners. The R-matrix is well settled for two-body channels and a complete review is given by Lane and Thomas [2]. Its general idea is to split up the configuration space into an interior and exterior region, where the Schrödinger equation is solved separately. In the interior region one expands the wave function over known basis states and in the exterior region the solution is a combination of the asymptotic forms of Bessel or (for charged particles) Coulomb functions. Both solutions are connected at the borderline via suitable boundary conditions.

However, the inclusion of channels with three particles has not been established yet. Up to now three-body processes have been treated as small perturbations and have mostly been omitted. An approximation for three-body channels was given by Lane and Thomas in [3] in the frame of two particle R-matrix theory. They consider the three-body process as having two particles in the exit channel, where one of them has sufficient energy to decay into two fragments. Usually in two-particle R-matrix theory one transforms integrals over the interior region into an integral over a surface S. This is chosen to be drawn far enough out in configuration space and can be therefore expressed as a sum of channel surfaces S_c with a finite radius a_c, respectively, which do not overlap. For two bound fragments in the exit channels with localized wave functions, a_c can be assigned some finite value. However, if one of them disintegrates in two bodies, its wave function becomes delocalized in configuration space and one is faced with the problem of defining a finite matching radius a_c. At that point approximations have to be introduced. One demands that the scattering wave function of the disintegrating fragment is (negligibly) small in all unbound channels so that a_c can be chosen to be finite. This implies an extended lifetime of the decaying body which turns the three-body break-up process into two successive two-body break-up processes. In that manner three-body decay processes can be covered by two-body R-matrix theory. The formalism only has to be extended to the occurrence of scattering wave functions in the exit channel which must be chosen to fulfill certain orthogonality conditions. This model of successive decay was successfully applied to three-body reactions but even to processes with up to seven reaction products in the exit channel [4]. However, this way does not really provide a satisfying solution for three-body break-up processes because of approximations. In 1976 Walter Glöckle suggested a way to solve the three-body problem in the frame of R-matrix theory for three *identical* particles [6] based on the theory of Faddeev [7]. Outgoing from the Faddeev equations in coordinate space and the asymptotic form of the Faddeev amplitudes, he deduces a set of four equations for the three-body on-shell T-matrix elements and the expansion coefficients of the interior wave functions. The scattering process is therefore treated in the sense of quantum mechanical coherence and is no longer considered to run sequentially. Glöckle's work will be the foundation of this thesis.

After a theoretical introduction to three-body scattering theory and Faddeev equations in Section 2, we will study and comment Glöckle's ideas and present more detailed derivations of the various results. This, together with a short discussion about the relation between T-matrix elements and the experimentally accessible cross section will be covered in Section 3.2. The main goal of the thesis, however, will be the generalization to a three-body R-matrix theory for (three) arbitrary particles. In Section 4 we will derive generic expressions for the three Faddeev components and their asymptotics in various orders. Finally we will establish a set of four equations by making use of a three-body R-matrix method. From these equations one should be able to determine the essential T-matrix elements that enter into the cross section.

2 Theoretical background

The content of this section will essentially follow [8]. First, we will give a short overview of three particle systems in general. The main part then will be the derivation of the Faddeev equations for various operators and the scattering states, which will be the foundation for the following sections.

2.1 Three-body systems and the Lippmann-Schwinger equation

We consider a three-particle system in the entrance channel, which is composed of a bound state between two-particles and the third one moving freely. After a reaction took place, we have five possible exit channels, one elastic channel, three rearrangement channels, one break-up channel and a bound channel, which will be omitted. The two-particles j and k in the bound subsystems interact via a two-body potential $v_i = v(j,k)$, while particle i moves freely. Generally, two-particle operators that act in a two-particle subsystem are denoted by small letters, whereas three-particle operators are represented by capital letters (except for channel Hamilton operators). Vectors will be represented by bold letters. In natural Jacobi coordinates (which will be introduced later) the total Hamilton operator reads ($i = 1, 2, 3$)

$$H = \frac{\hat{\mathbf{p}}_i^2}{2\mu_i} + \frac{\hat{\mathbf{q}}_i^2}{2M_i} + v_1 + v_2 + v_3 \equiv h_0 + V\,, \tag{2.1}$$

where

$$h_0 = \frac{\hat{\mathbf{p}}_i^2}{2\mu_i} + \frac{\hat{\mathbf{q}}_i^2}{2M_i} \tag{2.2}$$

and

$$V = v_1 + v_2 + v_3\,. \tag{2.3}$$

The motion of the center of mass is trivial and thus neglected. $\mathbf{p}_i$ is the relative momentum between particles j and k (if they form a bound state, p_i will be complex) and $\mathbf{q}_i$ the momentum of particle i in the center of mass system of all three-particles. $\hat{\mathbf{p}}_i$ and $\hat{\mathbf{q}}_i$ are the corresponding momentum operators. For the total energy of the three-body system both relative motions are added up and yield

$$E = \frac{p_i^2}{2\mu_i} + \frac{q_i^2}{2M_i}\,, \tag{2.4}$$

The reduced masses are

$$\mu_i = \frac{m_j m_k}{m_j + m_k} \qquad\qquad M_i = \frac{m_i(m_j + m_k)}{m_i + m_j + m_k}\,. \tag{2.5}$$

There are channel Hamilton operators for each channel,

$$h_\alpha = \frac{\hat{\mathbf{p}}_\alpha^2}{2\mu_\alpha} + \frac{\hat{\mathbf{q}}_\alpha^2}{2M_\alpha} + v_\alpha\,. \tag{2.6}$$

with the asymptotic channel states as eigenfunctions,

$$h_\alpha|\phi_{\alpha m}\rangle = E_\alpha|\phi_{\alpha m}\rangle\,. \tag{2.7}$$

They are related to the total Hamilton operator according to

$$H = h_\alpha + \overline{V}_\alpha\,, \tag{2.8}$$

with the definition

$$\overline{V}_\alpha = V - v_\alpha = \sum_{\alpha\neq\gamma} v_\gamma\,. \tag{2.9}$$

In each channel there is an interaction between two-particles, which is expressed by the respective potentials v_α, that are identical to v_i from above. In the asymptotic area of the break-up channel all particles are free, there is no interaction between any of them and thus

$$v_0 \equiv 0\,. \tag{2.10}$$

This is valid since nuclear forces act over very short distances only ($\approx 1\,\mathrm{fm}$). The problem of charged particles with a Coulomb interaction of infinite range is not treated in this thesis.

The essential equation of scattering theory is the Lippmann-Schwinger equation. We now want to derive it for the three-particle case via the resolvent $G(z)$, with $z = E \pm \mathrm{i}\epsilon$. The full resolvent of the three-particle system $G(z)$ is defined as

$$G(z) \equiv (z - H)^{-1}\,. \tag{2.11}$$

We get two equations for $G(z)$ using the channel resolvent $g_\alpha(z) = (z - h_\alpha)^{-1}$,

$$G(z) = g_\alpha(z) + g_\alpha(z)\overline{V}_\alpha G(z) = g_\alpha(z) + G(z)\overline{V}_\alpha g_\alpha(z)\,. \tag{2.12}$$

They can be verified by multiplying for instance the second equation in (2.12) by $G^{-1}(z)$ from the left and using the identity

$$g_\alpha^{-1}(z) - G^{-1}(z) = z - h_\alpha - z - H = \overline{V}_\alpha\,, \tag{2.13}$$

which yields

$$\begin{aligned} \mathbb{1} &= G^{-1}(z)g_\alpha(z) + \overline{V}_\alpha g_\alpha(z) \\ \mathbb{1} &= (g_\alpha^{-1}(z) - \overline{V}_\alpha)g_\alpha(z) + \overline{V}_\alpha g_\alpha(z) = \mathbb{1}\,. \end{aligned} \tag{2.14}$$

The scattering state in channel α is defined as

$$|\psi_{\alpha m}^{(\pm)}\rangle = \lim_{\epsilon\to 0} \pm\mathrm{i}\epsilon G(E \pm \mathrm{i}\epsilon)|\phi_{\alpha m}\rangle\,. \tag{2.15}$$

It is a three-particle wave packet with a subsystem of two-particle being in their m^{th} bound state and the third one moving freely. Inserting the first resolvent equation (2.12) into Eq. (2.15) leads, after executing the limits, to the Lippmann-Schwinger equation for a three-particle scattering state in channel α

$$|\psi^{(\pm)}_{\alpha m}\rangle = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_\alpha(z)|\phi_{\alpha m}\rangle + \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_\alpha(z)\overline{V}_\alpha G(z)|\phi_{\alpha m}\rangle = |\phi_{\alpha m}\rangle + g_\alpha(E\pm \mathrm{i}0)\overline{V}_\alpha|\psi^{(\pm)}_{\alpha m}\rangle\,. \tag{2.16}$$

We used the fact that $|\phi_{\alpha m}\rangle$ is an eigenstate of h_α and thus

$$\lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_\alpha(z)|\phi_{\alpha m}\rangle = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon (z-h_\alpha)^{-1}|\phi_{\alpha m}\rangle = \lim_{\epsilon\to 0} \frac{\pm \mathrm{i}\epsilon}{E\pm \mathrm{i}\epsilon - E_\alpha}|\phi_{\alpha m}\rangle = |\phi_{\alpha m}\rangle\,.$$

However, this equation exhibits a problem since it is not uniquely solvable. The reason is that the homogeneous equation

$$|\psi^{(\pm)}_{\alpha m}\rangle = g_\alpha(E\pm \mathrm{i}0)\overline{V}_\alpha|\psi^{(\pm)}_{\alpha m}\rangle \tag{2.17}$$

has non-trivial solutions in the region of scattering energies, where $E > 0$. This can be shown by writing down the Lippmann-Schwinger equation (2.16) for the scattering state of another channel $\beta \neq \alpha$,

$$|\psi^{(\pm)}_{\beta n}\rangle = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_\alpha(z)|\phi_{\beta n}\rangle + \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_\alpha(z)\overline{V}_\alpha G(z)|\phi_{\beta n}\rangle = g_\alpha(E\pm \mathrm{i}0)\overline{V}_\alpha|\psi^{(\pm)}_{\beta n}\rangle\,. \tag{2.18}$$

Since $|\phi_{\beta n}\rangle$ is not an eigenstate of h_α, $g_\alpha(z)|\phi_{\beta n}\rangle$ remains finite for ϵ approaching 0. Hence, what remains after performing the limit $\epsilon \to 0$ in Eq. (2.18), is the solution of the homogeneous equation

$$|\psi^{(\pm)}_{\beta n}\rangle = g_\alpha(E\pm \mathrm{i}0)\overline{V}_\alpha|\psi^{(\pm)}_{\beta n}\rangle\,. \tag{2.19}$$

It is an additional solution to $|\psi^{(\pm)}_{\alpha m}\rangle$ and can be added to it. In the two-particle case, there exist non-trivial solutions of the homogeneous Lippmann-Schwinger equation too. However, these solutions are found at discrete binding energies of the two-particle system ($E_{bind} < 0$), not in the positive energy region where scattering takes place.

There are further equations beside the Lippmann-Schwinger equation [9], which are satisfied by the scattering state $|\psi^{(\pm)}_{\alpha m}\rangle$, They result from inserting the second resolvent equation of (2.12) for $G(z)$, but now for a different channel than α, like β,

$$\begin{aligned}|\psi^{(+)}_{\alpha m}\rangle &= \lim_{\epsilon\to 0} \mathrm{i}\epsilon G(E+\mathrm{i}\epsilon)|\phi_{\alpha m}\rangle = \lim_{\epsilon\to 0} \mathrm{i}\epsilon g_\beta(E+\mathrm{i}\epsilon)|\phi_{\alpha m}\rangle + \lim_{\epsilon\to 0} \mathrm{i}\epsilon g_\beta(E+\mathrm{i}\epsilon)\overline{V}_\beta G(E+\mathrm{i}\epsilon)|\phi_{\alpha m}\rangle \\ &= \lim_{\epsilon\to 0} \frac{\mathrm{i}\epsilon}{E+\mathrm{i}\epsilon - h_\beta}|\phi_{\alpha m}\rangle + g_\beta(E+\mathrm{i}0)\overline{V}_\beta|\psi^{(+)}_{\alpha m}\rangle\,.\end{aligned} \tag{2.20}$$

The first term vanishes since $|\phi_{\alpha m}\rangle$ is not an eigenstate of h_β. Hence, the denominator remains finite while the numerator approaches to 0 in the. Finally, in the limit $\epsilon \to 0$ the product $g_\beta|\phi_{\alpha m}\rangle$ vanishes, which is known as the Lippmann identity. A similar equation is obtained by using the γ-resolvent.

Glöckle found out that adding these two equations to the Lippmann-Schwinger equation,

$$\begin{aligned}
|\psi^{(+)}_{\alpha m}\rangle &= |\phi_{\alpha m}\rangle + g_\alpha(E+\mathrm{i}0)\overline{V}_\alpha|\psi^{(+)}_{\alpha m}\rangle \\
|\psi^{(+)}_{\alpha m}\rangle &= \qquad\qquad g_\beta(E+\mathrm{i}0)\overline{V}_\beta|\psi^{(+)}_{\alpha m}\rangle \\
|\psi^{(+)}_{\alpha m}\rangle &= \qquad\qquad g_\gamma(E+\mathrm{i}0)\overline{V}_\gamma|\psi^{(+)}_{\alpha m}\rangle
\end{aligned} \tag{2.21}$$

the scattering solution $|\psi^{(+)}_{\alpha m}\rangle$ becomes unique [5]. These additional equations introduce physical boundary conditions to the Lippmann-Schwinger equation which guarantee that there are no incoming waves in channels β and γ. In the the break-up channel the behavior of $|\psi^{(+)}_{\alpha m}\rangle$ is determined by each of the three equations (2.21). Alternatively one can use the form (2.20) with $\beta = 0$, to describe $|\psi^{(+)}_{\alpha m}\rangle$ in the break-up channel,

$$|\psi^{(+)}_{\alpha m}\rangle = G_0\overline{V}_0|\psi^{(+)}_{\alpha m}\rangle = G_0 V|\psi^{(+)}_{\alpha m}\rangle\,. \tag{2.22}$$

This state again guarantees a purely outgoing wave in the break-up channel [9]. Moreover, the structure of (2.22) gives rise to a decomposition of $|\psi^{(+)}_{\alpha m}\rangle$ into components $|\psi^{(+)}_{\alpha m}\rangle_i$,

$$|\psi^{(+)}_{\alpha m}\rangle = G_0 V|\psi^{(+)}_{\alpha m}\rangle = \sum_{i=1}^{3} G_0 V_i|\psi^{(+)}_{\alpha m}\rangle_i\,, \tag{2.23}$$

which are called Faddeev components of the scattering wave function.

However, there are still problems remaining. The integral kernel of Eq. (2.16), $g_\alpha\overline{V}_\alpha$, and the integral kernels of the equations in (2.21) do not have a finite Schmidt norm (see below) and they are not compact. Latter is caused by the occurrence of delta functions in the kernel, which in a graphical representation appear as disconnected parts of the system, that should not appear in useful integral equations. The delta function arises from the fact that the channel resolvent g_α acts in the two-particle subsystem of the three-particle system, and does not affect particle α. This can be expressed by writing down the matrix elements of the resolvent (bold letters represent vectors)

$$\langle\mathbf{p}_\alpha\mathbf{q}_\alpha|g_\alpha(z)|\mathbf{p}'_\alpha\mathbf{q}'_\alpha\rangle = \delta(\mathbf{q}_\alpha - \mathbf{q}'_\alpha)\langle\mathbf{p}_\alpha|\hat{g}_\alpha(z - \frac{q_\alpha^2}{2M_\alpha})|\mathbf{p}'_\alpha\rangle\,. \tag{2.24}$$

Here, $\hat{g}_\alpha$ is a two-particle operator living in two-particle space, while g_α is a two-particle operator in three-particle space.

Faddeev was the first to realize these problems, which indicated him to look for new equations, the so-called Faddeev equations, subject of the following subsections.

2.2 Faddeev equations for the T-operator

We consider the three-particle T-operator,

$$T(z) = V + VG(z)V \tag{2.25}$$

and the three-particle resolvent

$$G(z) = g_0(z) + g_0(z)T(z)g_0(z)\,. \tag{2.26}$$

Combining them yields two integral equations for the T-operator, i.e.

$$\begin{aligned} T(z) &= V + V g_0(z) T(z)\,, \\ T(z) &= V + T(z) g_0(z) V\,. \end{aligned} \tag{2.27}$$

Faddeev suggested to split the T-operator into three components,

$$T_i = v_i + v_i g_0 T\,, \tag{2.28}$$

where $V = v_1 + v_2 + v_3$ and thus $T = T_1 + T_2 + T_3$. However, the integral kernel remains the same as before and is still non compact. We can arrange the equations for the three components in matrix from

$$\begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} + \begin{pmatrix} v_1 & v_1 & v_1 \\ v_2 & v_2 & v_2 \\ v_3 & v_3 & v_3 \end{pmatrix} g_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix}\,. \tag{2.29}$$

In the following some manipulations to this matrix equation are performed in order to make the integral kernel less singular. We pick out the first line of the matrix equation

$$T_1 = v_1 + v_1 g_0 (T_1 + T_2 + T_3) \tag{2.30}$$

or equivalent

$$(1 - v_1 g_0) T_1 = v_1 + v_1 g_0 (T_2 + T_3)\,. \tag{2.31}$$

Next, we multiply this equation by $(1 - v_1 g_0)^{-1}$ from the left which leads to

$$T_1 = (1 - v_1 g_0)^{-1} v_1 + (1 - v_1 g_0)^{-1} v_1 g_0 (T_2 + T_3)\,, \tag{2.32}$$

or

$$T_1 = t_1 + t_1 g_0 (T_2 + T_3)\,, \tag{2.33}$$

with the two-particle t-operators

$$t_i = (1 - v_i g_0)^{-1} v_i\,, \tag{2.34}$$

acting in the three-particle space. The same procedure can be carried out for the second and third line and we end up with the matrix equation

$$\begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} 0 & t_1 & t_1 \\ t_2 & 0 & t_2 \\ t_3 & t_3 & 0 \end{pmatrix} g_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} . \tag{2.35}$$

These are the Faddeev equations for the T-matrix. They can be alternatively written as

$$T_i(z) = t_i(z) + \sum_{i=1}^{3} F_{ij}(z) g_0(z) T_j(z) \tag{2.36}$$

with the Faddeev operator

$$F_{ij}(z) = (1 - \delta_{ij}) t_i(z) . \tag{2.37}$$

The potentials v_i have been totally replaced by the two-particle operators t_i acting in the three-particle space. Two particle operators, like t_i that act only in subsystem i, always enter off-shell into three-body scattering amplitudes because of the energy shift $z - q_i^2/2M_i$ in subsystem i. As a consequence, there is more information contained in three-particle scattering data than in two-particle data alone. Additionally, when performing the operator product $t_i g_0 T_j$ one has to integrate over all intermediate states $|\mathbf{p}_i'\rangle$ and $|\mathbf{q}_i'\rangle$, where

$$\frac{p_i^2}{2\mu_i} \neq z - \frac{q_i'^2}{2M_i} \neq \frac{p_i'^2}{2\mu_i} . \tag{2.38}$$

The kernel of Eqs. (2.35) and (2.36), $t_i g_0 T_j$, is still not compact and does not have a finite Schmidt norm. This is due to the exclusive action of t_i in subsystem i, which causes δ-functions occurring in the matrix elements,

$$\langle \mathbf{p}_i \mathbf{q}_i | t_i(z) | \mathbf{p}_i' \mathbf{q}_i' \rangle = \delta(\mathbf{q}_\alpha - \mathbf{q}_\alpha') \langle \mathbf{p}_i | \hat{t}_i (z - \frac{q_i^2}{2M_i}) | \mathbf{p}_i' \rangle . \tag{2.39}$$

The existence of the Schmidt norm of an operator $K(\mathbf{r}, \mathbf{r}')$ is defined as

$$\|K\|_S = \left[\mathrm{Tr}(K^\dagger K)\right]^{1/2} = \left[\iint \mathrm{d}\mathbf{r0}\, \mathrm{d}\mathbf{r}' |K(\mathbf{r}, \mathbf{r}')|^2\right]^{1/2} , \tag{2.40}$$

and is a sufficient condition for compactness of the integral kernel. Latter is an important feature of the kernel as it is a necessary condition to enable the Fredholm theory and other methods of integral equation theory to be applied. After a first iteration of Eq. (2.35), not carried out here, there occur operator products such as $t_i g_0 t_j$ with $i \neq j$. Such a product implies an integration over intermediate energy states, where the δ-functions disappear and the particles get linked together. Further problems and details are treated in [8], however, we can proceed using the form (2.36) of the Faddeev equations for the T-operator. If we continue iterating Eq. (2.35), we get the Neumann series of the Faddeev equations, which is [8],

$$\underline{T}(z) = \sum_{\nu=0}^{\infty} \underline{t}(z) \left(\underline{\underline{F}}(z) g_0(z) \underline{t}(z) \right)^{\nu} , \tag{2.41}$$

where doubly underlined quantities represent matrices and singly underlined quantities vectors. The Neumann series and its graphical representation (see [8]) reveal the meaning of the Faddeev equations. The Faddeev equations describe the three-particle scattering process as a two-body multiple scattering process, where the individual two-body scattering occurs on-shell or off-shell.

In the next step we will derive Faddeev equations for the three-particle resolvent $G_i(z)$ and the scattering wave function $|\psi^{\pm}_{\alpha m}\rangle$.

2.3 Faddeev equations for the resolvent and scattering states

We start with the resolvent $G(z)$ from Eq. (2.26) and replace the operator T by the sum of its three components T_i (2.2),

$$G(z) = g_0(z) + \sum_{i=1}^{3} g_0(z) T_i(z) g_0(z) \,. \tag{2.42}$$

With the definition of components $G_i(z)$,

$$G_i(z) = g_0(z) T_i(z) g_0(z) \tag{2.43}$$

we can rewrite Eq. (2.42)

$$G(z) = g_0(z) + \sum_{i=1}^{3} G_i(z) \,. \tag{2.44}$$

Equations that determine $G_i(z)$ can be obtained by inserting the Faddeev equations (2.36) for the T-operator into Eq. (2.43) (omitting the argument z of the resolvents and operators),

$$G_i = g_0 t_i g_0 + g_0 \sum_{j=1}^{3} F_{ij} g_0 T_j g_0 \,. \tag{2.45}$$

We proceed by including a relation that follows form extending the resolvent equation in two-particle space

$$g(z) = g_0(z) + g_0(z) t(z) g_0(z) \tag{2.46}$$

into three-particle space,

$$g_0 t_i g_0 = g_i - g_0 \,. \tag{2.47}$$

Then,

$$G_i(z) = g_i(z) - g_0(z) + \sum_{j=1}^{3} F_{ij} g_0 T_j g_0 \tag{2.48}$$

and with Eq. (2.43) we obtain

$$G_i(z) = g_i(z) - g_0(z) + \sum_{j=1}^{3} g_0(z) F_{ij}(z) G_j(z)\,. \tag{2.49}$$

Let us now find Faddeev equations for the scattering state

$$|\psi^{(\pm)}_{\alpha m}\rangle = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon G(E \pm \mathrm{i}\epsilon)|\phi_{\alpha m}\rangle \tag{2.50}$$

by inserting the splitting of the resolvent (2.44), which yields

$$|\psi^{(\pm)}_{\alpha m}\rangle = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_0(E \pm \mathrm{i}\epsilon)|\phi_{\alpha m}\rangle + \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon \sum_{i=1}^{3} G_i(E \pm \mathrm{i}\epsilon)|\phi_{\alpha m}\rangle\,. \tag{2.51}$$

We define

$$|\chi^{(\pm)}_{i\alpha m}\rangle = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon g_i(E \pm \mathrm{i}\epsilon)|\phi_{\alpha m}\rangle \tag{2.52}$$

and

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon G_i(E \pm \mathrm{i}\epsilon)|\phi_{\alpha m}\rangle\,, \tag{2.53}$$

with $i = 1, 2, 3$. The state $|\chi^{(\pm)}_{i\alpha m}\rangle$ with $\alpha \neq 0$ can be simplified by performing the limit $\epsilon \to 0$,

$$|\chi^{(\pm)}_{i\alpha m}\rangle = \lim_{\epsilon\to 0} \frac{\pm \mathrm{i}\epsilon}{E \pm \mathrm{i}\epsilon - h_i}|\phi_{\alpha m}\rangle = \delta_{i\alpha}|\phi_{\alpha m}\rangle\,, \qquad i = 0, 1, 2, 3\,, \tag{2.54}$$

which is true since $|\phi_{\alpha m}\rangle$ is an eigenfunction of h_i if $i = \alpha$. $\alpha \neq 0$ means an incoming state consisting of a bound pair and one particle moving freely. This case will be considered in the following. For $\alpha = 0$, which describes an incoming state consisting of three free particles, we get different results for $|\chi^{(\pm)}_{i\alpha m}\rangle$, which, however, will not concern us further. As a consequence the scattering state is split into components

$$|\psi^{(\pm)}_{\alpha m}\rangle = |\chi^{(\pm)}_{0\alpha m}\rangle + \sum_{i=1}^{3} |\psi^{(\pm)}_{\alpha m}\rangle_i\,. \tag{2.55}$$

With the Faddeev equations for the resolvent (2.49), these components become

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = \lim_{\epsilon\to 0} \pm \mathrm{i}\epsilon \left[g_i(E \pm \mathrm{i}\epsilon) - g_0(E \pm \mathrm{i}\epsilon) + \sum_{j=1}^{3} g_0(E \pm \mathrm{i}\epsilon) F_{ij}(E \pm \mathrm{i}\epsilon) G_j(E \pm \mathrm{i}\epsilon) \right] |\phi_{\alpha m}\rangle\,. \tag{2.56}$$

For an incoming state consisting of a bound pair and one particle moving freely we obtain

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = \delta_{i\alpha}|\phi_{\alpha m}\rangle + \sum_{j=1}^{3} g_0(E \pm \mathrm{i}0) F_{ij}(E \pm \mathrm{i}0) |\psi^{(\pm)}_{\alpha m}\rangle_j \tag{2.57}$$

and the total scattering wave function is a coherent sum of the three Faddeev components,

$$|\psi_{\alpha m}^{(\pm)}\rangle = \sum_{i=1}^{3} |\psi_{\alpha m}^{(\pm)}\rangle_i \,. \tag{2.58}$$

These are the Faddeev equations for the scattering state that we will use in the following.

3 The Glöckle R-matrix approach to the three-body problem

3.1 Introduction

In the first part of this section, we follow Glöckle's way to derive a set of equations for the three-body on-shell T-matrix elements by the R-matrix method. His idea will be the basis for our generalization of the three-body R-matrix approach to different masses of the three interacting particles. However, we present a more detailed derivation of the results provided in [6] before generalizing them to arbitrary particle masses.

The total scattering wave function $\Psi^{(+)}$ is decomposed according to Faddeev [7] into three wave functions which in coordinate space representation are

$$\Psi^{(+)} = \psi_1(r_1, R_1) + \psi_2(r_2, R_2) + \psi_3(r_3, R_3), \tag{3.1}$$

where $\mathbf{r}_i$ and $\mathbf{R}_i$, $i = 1, 2, 3$ denote Jacobi coordinates (bold letters denote vectors). The three sets of Jacobi coordinates are defined as

$$\mathbf{r}_1 = \mathbf{x}_2 - \mathbf{x}_3\,, \qquad \mathbf{R}_1 = \mathbf{x}_1 - \frac{m_2\mathbf{x}_2 + m_3\mathbf{x}_3}{m_2 + m_3}\,, \tag{3.2}$$

$$\mathbf{r}_2 = \mathbf{x}_3 - \mathbf{x}_1\,, \qquad \mathbf{R}_2 = \mathbf{x}_2 - \frac{m_3\mathbf{x}_3 + m_1\mathbf{x}_1}{m_1 + m_3}\,, \tag{3.3}$$

$$\mathbf{r}_3 = \mathbf{x}_1 - \mathbf{x}_2\,, \qquad \mathbf{R}_3 = \mathbf{x}_3 - \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}\,, \tag{3.4}$$

where $\mathbf{x}_i$ represent Cartesian coordinates. The different sets of Jacobi coordinates are illustrated in Fig. 1

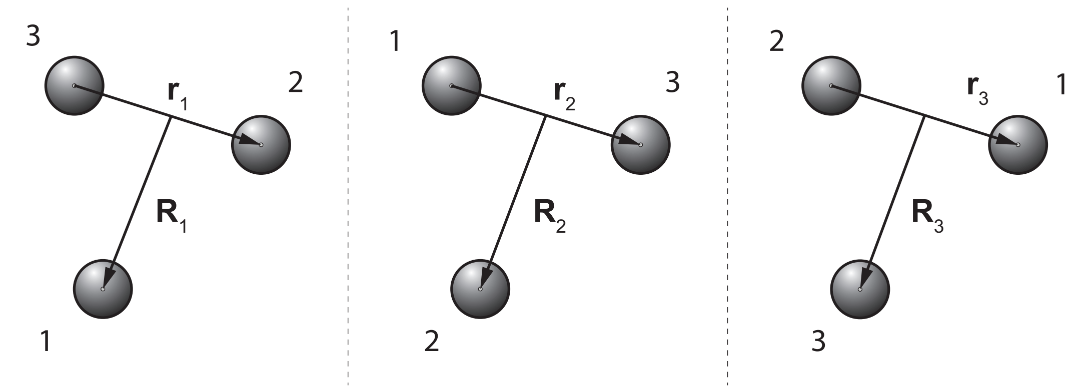

Figure 1: Definition of Jacobi coordinates

The Faddeev equation for the scattering wave function (2.57) reads

$$
\begin{aligned}
|\psi^{(\pm)}_{\alpha m}\rangle_i = \delta_{i\alpha}|\phi_{\alpha m}\rangle + \sum_{j=1}^{3} g_0 F_{ij}|\psi^{(\pm)}_{\alpha m}\rangle_j = \delta_{i\alpha}|\phi_{\alpha m}\rangle + \sum_{j=1}^{3} g_0(1-\delta_{ij})t_i|\psi^{(\pm)}_{\alpha m}\rangle_j \\
= \delta_{i\alpha}|\phi_{\alpha m}\rangle + \sum_{j(\neq i)=1}^{3} g_0 t_i|\psi^{(\pm)}_{\alpha m}\rangle_j \,,
\end{aligned}
\tag{3.5}
$$

with

$$
|\psi^{(\pm)}_{\alpha m}\rangle = \sum_{i=1}^{3} |\psi^{(\pm)}_{\alpha m}\rangle_i \,. \tag{3.6}
$$

Here we used the identity $F_{ij} = (1-\delta_{ij})t_i$. From (2.34) it follows

$$
t_i = (1 - v_i g_0)^{-1} v_i \tag{3.7}
$$

and after a slight manipulation of the resolvent equation,

$$
g_i(z) = g_0(z) + g_i(z) v_i g_0(z) \,, \tag{3.8}
$$

one arrives at

$$
g_i = (1 - v_i g_0)^{-1} g_0 \,. \tag{3.9}
$$

Dividing Eq. (3.7) by Eq. (3.9) we get

$$
\frac{t_i}{g_i} = \frac{v_i}{g_0} \Rightarrow g_0 t_i = g_i v_i \tag{3.10}
$$

and Eq. (3.5) can be rewritten

$$
|\psi^{(\pm)}_{\alpha m}\rangle_i = \delta_{i\alpha}|\phi_{\alpha m}\rangle + g_i v_i \sum_{j(\neq i)=1}^{3} |\psi^{(\pm)}_{\alpha m}\rangle_j \,. \tag{3.11}
$$

First, following Glöckle [6, 9] we restrict ourselves to the simplified model of three identical spinless (bosonic) particles with s-wave interaction only. This assumption is primarily valid in the energy regime near the break-up threshold. In Sec. 4 we generalize the results for scattering of three distinguishable particles with different masses also interacting by s-wave interaction only. In the following, we use the coordinate space representations of the various physical scattering wave functions $|\psi^{(+)}_{\alpha m}\rangle_i$ and suppress the indices α and m

$$
\psi_i(\mathbf{r}_j, \mathbf{R}_j) \equiv {}_i\langle \mathbf{r}_j \mathbf{R}_j | \psi^{(+)}_{\alpha m}\rangle_i \,. \tag{3.12}
$$

The index $i = 1, 2, 3$ and j denote the Faddeev component and a certain set of Jacobi coordinates, respectively. In the next sections we change the notation for two-particle Green's functions and two-body potentials from small to capital letters while leaving their definitions unchanged and set $\hbar \equiv 1$.

3.2 Three interacting identical spinless bosons

In this subsection we assume equal masses $m_1 = m_2 = m_3$ and units $m_i = 1$, $\hbar = 1$.

Further we define permutation operators P_{ij} that interchange particles i and j. Following [9], the definition of the Faddeev components (2.23) leads to the relationships

$$\begin{aligned} \psi_2(\mathbf{r}_2, \mathbf{R}_2) &= {}_2\langle \mathbf{r}_2\mathbf{R}_2|G_0 V_2 \varPsi\rangle = {}_2\langle \mathbf{r}_2\mathbf{R}_2|P_{12}P_{23}|G_0 V_1 \varPsi\rangle = {}_2\langle \mathbf{r}_2\mathbf{R}_2|P_{12}P_{23}|\psi_1\rangle \\ &= {}_1\langle \mathbf{r}_2\mathbf{R}_2|\psi_1\rangle = \psi_1(\mathbf{r}_2, \mathbf{R}_2) \end{aligned} \tag{3.13}$$

In the second and last equality of Eq. (3.13) we make use of the fact that the bosonic scattering wave function is symmetric under permutation of particles. Additionally we use the invariance of the Green's function G_0 under permutation of particles and the identity $P_{12}P_{23}V_1 = V_2$. In the third step we reinsert the definition of the Faddeev components. Analogously we get

$$\begin{aligned} \psi_3(\mathbf{r}_3, \mathbf{R}_3) &= {}_3\langle \mathbf{r}_3\mathbf{R}_3|G_0 V_3 \varPsi\rangle = {}_3\langle \mathbf{r}_3\mathbf{R}_3|P_{13}P_{23}|G_0 V_1 \varPsi\rangle = {}_3\langle \mathbf{r}_3\mathbf{R}_3|P_{13}P_{23}|\psi_1\rangle \\ &= {}_1\langle \mathbf{r}_3\mathbf{R}_3|\psi_1\rangle = \psi_1(\mathbf{r}_3, \mathbf{R}_3) \end{aligned} \tag{3.14}$$

As indicated in the last two equations, all three Faddeev components have the same functional form, if they are expressed in Jacobi coordinates. Consequently, instead of three coupled Faddeev equations, we obtain three separate equations that can be solved independently. For $\psi_1(\mathbf{r}_1, \mathbf{R}_1)$, for instance, according to (3.11), we obtain [9]

$$\psi_1(\mathbf{r}_1, \mathbf{R}_1) = \phi_1(\mathbf{r}_1, \mathbf{R}_1) + \int \mathrm{d}^3 r'_1 \int \mathrm{d}^3 R'_1 \langle \mathbf{r}_1\mathbf{R}_1|G_1|\mathbf{r}'_1\mathbf{R}'_1\rangle V_1(r'_1)[\psi_1(\mathbf{r}'_2, \mathbf{R}'_2) + \psi_1(\mathbf{r}'_3, \mathbf{R}'_3)]\,. \tag{3.15}$$

From a practical point of view, one would solve Eq. (3.15) only and substitute the coordinates in the result in order to obtain the solution for the other Faddeev components $\psi_1(\mathbf{r}_2, \mathbf{R}_2)$ and $\psi_1(\mathbf{r}_3, \mathbf{R}_3)$. So we can define $\psi_1(\mathbf{r}_1, \mathbf{R}_1) \equiv \psi(\mathbf{r}_1, \mathbf{R}_1)$, $\psi_1(\mathbf{r}_2, \mathbf{R}_2) \equiv \psi(\mathbf{r}_2, \mathbf{R}_2)$ and $\psi_1(\mathbf{r}_3, \mathbf{R}_3) \equiv \psi(\mathbf{r}_3, \mathbf{R}_3)$. The Jacobi coordinates now read

$$\begin{aligned} &\mathbf{r}_1 = \mathbf{x}_2 - \mathbf{x}_3 && \mathbf{r}_2 = \mathbf{x}_3 - \mathbf{x}_1 && \mathbf{r}_3 = \mathbf{x}_1 - \mathbf{x}_2 \\ &\mathbf{R}_1 = \mathbf{x}_1 - \frac{1}{2}(\mathbf{x}_2 + \mathbf{x}_3) && \mathbf{R}_2 = \mathbf{x}_2 - \frac{1}{2}(\mathbf{x}_3 + \mathbf{x}_1) && \mathbf{R}_3 = \mathbf{x}_3 - \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2)\,, \end{aligned} \tag{3.16}$$

which follow from Eqs. (3.2)- (3.4) for $m_1 = m_2 = m_3 = 1$.

The three-particle scattering wave function $\psi(\mathbf{r}_j, \mathbf{R}_j)$ can be separated into a radial and an angular part,

$$\psi(\mathbf{r}_j, \mathbf{R}_j) = 4\pi \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} i^{l+l'} R_{ll'}(r_j, R_j; k) \sum_{m=-l}^{l} Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{R}}_j) \sum_{m'=-l'}^{l'} Y_{l'm'}(\hat{\mathbf{r}}_j)\,, \tag{3.17}$$

where l denotes the angular momentum quantum number, m the magnetic quantum number and Y_{lm} the spherical harmonics. The wave number of the free relative motion of the single particle with respect to the bound pair with binding energy E_b is $k = \sqrt{\frac{4}{3}(E - E_b)}$. The radial function $R_{ll'}(r_j, R_j; k)$ is written as

$$R_{ll'}(r_j, R_j; k) = \frac{u_l(r_j, R_j; k)}{r_j R_j k} \,. \tag{3.18}$$

The inhomogeneous term $\phi_1(\mathbf{r}_1, \mathbf{R}_1)$ in Eq. (3.15) refers to the incoming flux in the entrance channel,

$$\begin{aligned} \phi_1(\mathbf{r}_1, \mathbf{R}_1) &= \Phi_b(\mathbf{r}_1) \cdot \psi(\mathbf{k}, \mathbf{R}_1) = \Phi_b(\mathbf{r}_1) \cdot \mathrm{e}^{i\mathbf{k}\mathbf{R}_1} \\ &= \frac{u_{l'}(r_1)}{r_1} Y_{l'm'}(\hat{\mathbf{r}}_1) \cdot 4\pi \sum_{l=0}^{\infty} i^l \frac{\hat{\jmath}_l(kR_1)}{kR_1} \sum_{m=-l}^{l} Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{R}}_1) \,, \end{aligned} \tag{3.19}$$

where $\hat{\jmath}_l(kR_1)$ are the spherical Bessel functions in Ricatti form. It describes the free relative motion of a single particle, represented by its wave function $\psi(\mathbf{k}, \mathbf{R}_1)$ and a bound pair of particles, expressed by the binding wave function $\Phi_b(\mathbf{r}_1)$. Latter is square integrable and normalized to 1, i.e. $\int \mathrm{d}^3 r_1 [\Phi_b(\mathbf{r}_1)]^2 = 1$, which provides a normalization condition for the binding wave function $u_{l'}(r_1)$,

$$\begin{aligned} 1 &= \int \mathrm{d}^3 r_1 [\Phi_b(\mathbf{r}_1)]^2 = \int \mathrm{d}^3 r_1 \left(\frac{u_{l'}(r_1)}{r_1} \right)^2 Y^*_{l'm'}(\hat{\mathbf{r}}_1) Y_{l'm'}(\hat{\mathbf{r}}_1) \\ &= \int_0^\infty \mathrm{d}r_1 \, r_1^2 \frac{[u_{l'}(r_1)]^2}{r_1^2} \underbrace{\int \mathrm{d}\hat{r}_1 Y^*_{l'm'}(\hat{\mathbf{r}}_1) Y_{l'm'}(\hat{\mathbf{r}}_1)}_{=1} \Rightarrow \int_0^\infty \mathrm{d}r_1 [u_{l'}(r_1)]^2 = 1 \,. \end{aligned} \tag{3.20}$$

The solution $u_{l'}(r_1)$ satisfies the equation

$$\left[-\frac{1}{2\mu_{23}} \left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} \right) + V(r) \right] u_l(r) = \left[-\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} \right) + V(r) \right] u_l(r) = E_b u_l(r) \,, \tag{3.21}$$

where

$$\mu_{23} = \frac{m_2 m_3}{m_2 + m_3} = \frac{1}{2} \tag{3.22}$$

is the reduced mass of the subsystem consisting of particles 2 and 3. In partial wave decomposition, Eq. (3.15) becomes

$$\begin{aligned}
&4\pi\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty} i^{l+l'}\frac{u_{ll'}(r_1,R_1;k)}{r_1R_1k}\sum_{m=-l}^{l}Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{R}}_1)\sum_{m'=-l'}^{l'}Y_{l'm'}(\hat{\mathbf{r}}_1)\\
=&\frac{u_{l'}(r_1)}{r_1}Y_{l'm'}(\hat{\mathbf{r}}_1)\cdot 4\pi\sum_{l=0}^{\infty}i^l\frac{\hat{\jmath}_l(kR_1)}{kR_1}\sum_{m=-l}^{l}Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{R}}_1)+\int \mathrm{d}\mathbf{r}'_1\mathrm{d}\mathbf{R}'_1\langle\mathbf{r}_1\mathbf{R}_1|G_1|\mathbf{r}'_1\mathbf{R}'_1\rangle V_1(r'_1)\\
&\times\Bigg[4\pi\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty} i^{l+l'}\frac{u_{ll'}(r_2,R_2;k)}{r_2R_2k}\sum_{m=-l}^{l}Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{R}}_2)\sum_{m'=-l'}^{l'}Y_{l'm'}(\hat{\mathbf{r}}_2)+\\
&4\pi\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty} i^{l+l'}\frac{u_{ll'}(r_3,R_3;k)}{r_3R_3k}\sum_{m=-l}^{l}Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{R}}_3)\sum_{m'=-l'}^{l'}Y_{l'm'}(\hat{\mathbf{r}}_3)\Bigg].
\end{aligned} \tag{3.23}$$

In order to get rid of inessential difficulties in further calculations we introduce simplifications. The first is the restriction to the state of total angular momentum $L = 0$. The partial-wave decomposition of the various incoming and scattering wave functions then contain the s-wave part of the two relative motions (particle 2 versus particle 3 and particle 1 versus the system of particles 2 and 3 in a bound or scattering state) only which means $l = l' = 0$. The potential $V(r_1)$ is also assumed to act only in the s-wave. Consequently, $\psi_1(\mathbf{r}_1,\mathbf{R}_1)$ and $\phi_1(\mathbf{r}_1,\mathbf{R}_1)$ depend on the magnitudes $r_1 = |\mathbf{r}_1|$ and $R_1 = |\mathbf{R}_1|$ only which leads to a dependence of the amplitudes under the integral in (3.15) of $r'_2 = |\mathbf{r}'_2|$, $R_2 = |\mathbf{R}'_2|$, $r'_3 = |\mathbf{r}'_3|$ and $R'_3 = |\mathbf{R}'_3|$. Relations between different sets of Jacobi coordinates are given by

$$\begin{aligned}
\mathbf{r}_2 &= -\frac{1}{2}\mathbf{r}_1 - \mathbf{R}_1 \qquad \mathbf{R}_2 = \frac{3}{4}\mathbf{r}_1 - \frac{1}{2}\mathbf{R}_1,\\
\mathbf{r}_3 &= -\frac{1}{2}\mathbf{r}_1 + \mathbf{R}_1 \qquad \mathbf{R}_3 = -\frac{3}{4}\mathbf{r}_1 - \frac{1}{2}\mathbf{R}_1\,.
\end{aligned} \tag{3.24}$$

It follows that

$$r_2(x) = \sqrt{\frac{1}{4}r_1^2 + R_1^2 + \mathbf{R}_1\mathbf{r}_1} = \sqrt{\frac{1}{4}r_1^2 + R_1^2 + R_1r_1x} \tag{3.25}$$

and

$$R_2(x) = \sqrt{\frac{9}{16}r_1^2 + \frac{1}{4}R_1^2 - \frac{3}{4}\mathbf{R}_1\mathbf{r}_1} = \sqrt{\frac{1}{4}R_1^2 + \frac{9}{16}r_1^2 - \frac{3}{4}R_1r_1x}\,. \tag{3.26}$$

where x is the cosine of the angle between $\mathbf{r}_1$ and $\mathbf{R}_1$. For $r_3(x)$ and $R_3(x)$ we get

$$r_3(x) = \sqrt{\frac{1}{4}r_1^2 + R_1^2 - \mathbf{R}_1\mathbf{r}_1} = \sqrt{\frac{1}{4}r_1^2 + R_1^2 - R_1r_1x} \tag{3.27}$$

and

$$R_3(x) = \sqrt{\frac{9}{16}r_1^2 + \frac{1}{4}R_1^2 + \frac{3}{4}\mathbf{R}_1\mathbf{r}_1} = \sqrt{\frac{1}{4}R_1^2 + \frac{9}{16}r_1^2 + \frac{3}{4}R_1r_1x}\,. \tag{3.28}$$

The magnitudes r_2, R_2, r_3 and R_3 depend on $x = \hat{\mathbf{r}}_1\cdot\hat{\mathbf{R}}_1$, the cosine of the angle between $\mathbf{r}_1$ and $\mathbf{R}_1$. Hence, the six-dimensional integral in Eq. (3.15) reduces to a three-dimensional one, because the integration over the remaining three angles Θ, Φ and ϕ becomes trivial under these simplifications

$(x' = \hat{\mathbf{r}}'_1 \cdot \hat{\mathbf{R}}'_1)$,

$$\begin{aligned}
&\int \mathrm{d}^3 r'_1 \int \mathrm{d}^3 R'_1 \langle \mathbf{r}_1 \mathbf{R}_1 | G_1 | \mathbf{r}'_1 \mathbf{R}'_1 \rangle V_1(r'_1) [\psi_1(\mathbf{r}'_2, \mathbf{R}'_2) + \psi_1(\mathbf{r}'_3, \mathbf{R}'_3)] \\
&= \int_0^{2\pi} \mathrm{d}\Phi \int_0^{\pi} \mathrm{d}\Theta \, \sin\Theta \int_0^{\infty} \mathrm{d}R'_1 \, R_1^{'2} \int_0^{2\pi} \mathrm{d}\theta \, \sin\theta \int_0^{2\pi} \mathrm{d}x' \int_0^{\infty} \mathrm{d}r'_1 \, r_1^{'2} \langle \mathbf{r}_1 \mathbf{R}_1 | G_1 | \mathbf{r}'_1 \mathbf{R}'_1 \rangle V_1(r'_1) \\
&\quad \times [\psi_1(\mathbf{r}'_2, \mathbf{R}'_2) + \psi_1(\mathbf{r}'_3, \mathbf{R}'_3)] \\
&\longrightarrow 8\pi^2 \int_0^{\infty} \mathrm{d}r_1 \, r_1^{'2} \int_0^{\infty} \mathrm{d}R_1 \, R_1^{'2} \int_{-1}^{1} \mathrm{d}x' \langle \mathbf{r}_1 \mathbf{R}_1 | G_1 | \mathbf{r}'_1 \mathbf{R}'_1 \rangle V_1(r'_1) [\psi_1(r'_2, R'_2)_{l=0} + \psi_1(r'_3, R'_3)_{l=0}] \,.
\end{aligned} \tag{3.29}$$

The wave functions in last line of Eq.(3.29) only contain the s-wave part of the relative motions. We have also changed the integrations variables from (r'_1, ϕ, θ) to $(r'_1, \phi', \eta = \phi - \theta)$ because the magnitudes r'_2, R'_2, r'_3 and R'_3 appearing as arguments of the wave functions under the integral, depend on the relative angle $\eta = \arccos x$ between $\mathbf{r}_1$ and $\mathbf{R}_1$.
We can also find the partial wave decomposition of the Green's function matrix element [10] in Eq. (3.23)

$$\begin{aligned}
&\langle \mathbf{r}_1 \mathbf{R}_1 | G_1 | \mathbf{r}'_1 \mathbf{R}'_1 \rangle = \langle r_1 R_1 | G_1 | r'_1 R'_1 \rangle \frac{1}{r_1 R_1 r'_1 R'_1} \sum_{\mu=-\lambda}^{\lambda} Y^*_{\lambda\mu}(\hat{\mathbf{r}}_1) Y_{\lambda\mu}(\hat{\mathbf{R}}_1) \sum_{\mu'=-\lambda'}^{\lambda'} Y^*_{\lambda'\mu'}(\hat{\mathbf{r}}'_1) Y_{\lambda'\mu'}(\hat{\mathbf{R}}'_1) \\
&= -2\mu_{1(23)} \sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} \frac{g_{\lambda\lambda'}(r_1, R_1, r'_1, R'_1; k)}{k} \frac{1}{r_1 R_1 r'_1 R'_1} \sum_{\mu=-\lambda}^{\lambda} Y^*_{\lambda\mu}(\hat{\mathbf{r}}_1) Y_{\lambda\mu}(\hat{\mathbf{R}}_1) \sum_{\mu'=-\lambda'}^{\lambda'} Y^*_{\lambda'\mu'}(\hat{\mathbf{r}}'_1) Y_{\lambda'\mu'}(\hat{\mathbf{R}}'_1) \,.
\end{aligned} \tag{3.30}$$

This is essentially the generalization of the Green's function for two free particles

$$G_0(\mathbf{r}, \mathbf{r}', k) = -\frac{1}{4\pi} \frac{\mathrm{e}^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = 2\mu \sum_{l=0}^{\infty} \frac{g_l(r, r')}{r r'} \sum_{m=-l}^{l} Y^*_{lm}(\hat{\mathbf{r}}) Y_{lm}(\hat{\mathbf{r}}') \,, \tag{3.31}$$

where

$$g_l(r, r') = -\frac{1}{k} \hat{j}_l(kr_<) \hat{h}_l^{(+)}(kr_>) \,, \tag{3.32}$$

with the spherical Bessel function $j_l(x) = \frac{\hat{j}_l(x)}{x}$ and the spherical Hankel function $h_l^{(+)}(x) = \frac{\hat{h}_l^{(+)}(x)}{x}$.
Inserting the results of Eqs. (3.29) and (3.30) into Eq. (3.23) and considering only s-waves in both

relative motions ($l = l' = \lambda = \lambda' = 0$), Eq. (3.23) reduces to

$$
\begin{aligned}
&4\pi\frac{u(r_1,R_1;k)}{r_1R_1k}\frac{1}{(4\pi)^{3/2}}\\
=&\frac{u_b(r_1)}{r_1}\sqrt{\frac{1}{4\pi}}4\pi\frac{\sin(kR_1)}{kR_1}\frac{1}{4\pi}+8\pi^2\int\limits_0^\infty \mathrm{d}r_1'\ r_1'^2\int\limits_0^\infty \mathrm{d}R_1'\ R_1'^2\int\limits_{-1}^{1}\mathrm{d}x'\ \langle r_1R_1|G_1|r_1'R_1'\rangle\frac{1}{r_1R_1r_1'R_1'}\frac{1}{(4\pi)^2}V_1(r_1')\\
&\times\left[4\pi\frac{u(r_2',R_2';k)}{r_2'R_2'k}\frac{1}{(4\pi)^{3/2}}+4\pi\frac{u(r_3',R_3';k)}{r_3'R_3'k}\frac{1}{(4\pi)^{3/2}}\right].
\end{aligned}
\tag{3.33}
$$

with $u_{l=0,l'=0}(r_1,R_1;k)\equiv u(r_1,R_1;k)$, the binding wave function $u_{l'=0}(r_1)\equiv u_b(r_1)$ and $Y_{l=0,m=0}=\sqrt{\frac{1}{4\pi}}$.

Comparing Eq. (3.25) with Eq. (3.27) and Eq. (3.26) with Eq. (3.28) we conclude that

$$
r_3(x) = r_2(-x) \tag{3.34}
$$

and

$$
R_3(x) = R_2(-x)\,. \tag{3.35}
$$

These relations simplify the integral in Eq. (3.33) significantly. Considering the integration over x only, it turns out that the sum under the integral can be written as one single term,

$$
\begin{aligned}
&\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_2(x),R_2(x);k)}{r_2(x)R_2(x)}+\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_3(x),R_3(x);k)}{r_3(x)R_3(x)}\\
&=\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_2(x),R_2(x);k)}{r_2(x)R_2(x)}+\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_2(-x),R_2(-x);k)}{r_2(-x)R_2(-x)}\\
&=\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_2(x),R_2(x);k)}{r_2(x)R_2(x)}+\int\limits_{1}^{-1}(-\mathrm{d}y)\frac{u(r_2(y),R_2(y);k)}{r_2(y)R_2(y)}\\
&=\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_2(x),R_2(x);k)}{r_2(x)R_2(x)}+\int\limits_{-1}^{1}\mathrm{d}y\frac{u(r_2(y),R_2(y);k)}{r_2(y)R_2(y)}\\
&=2\int\limits_{-1}^{1}\mathrm{d}x\frac{u(r_2(x),R_2(x);k)}{r_2(x)R_2(x)}\,,
\end{aligned}
\tag{3.36}
$$

where we substituted $y = -x \Rightarrow \mathrm{d}y = -\mathrm{d}x$. Finally Eq. (3.33) becomes

$$\begin{aligned}
&\frac{u(r_1,R_1;k)}{r_1R_1k}\frac{1}{(4\pi)^{1/2}} = \frac{u_b(r_1)}{r_1}\frac{1}{(4\pi)^{1/2}}\frac{\sin(kR_1)}{kR_1} \\
&+ 8\pi^2\int_0^\infty \mathrm{d}r_1'\int_0^\infty \mathrm{d}R_1'\ \langle r_1R_1|G_1|r_1'R_1'\rangle\frac{r_1'^2R_1'^2}{r_1R_1r_1'R_1'}\frac{1}{(4\pi)^2}V_1(r_1')\int_{-1}^{1}\mathrm{d}x'\ 2\frac{u(r_2',R_2';k)}{r_2'R_2'k}\frac{1}{(4\pi)^{1/2}} \\
&= \frac{u_b(r_1)}{r_1}\frac{1}{(4\pi)^{1/2}}\frac{\sin(kR_1)}{kR_1} + 8\pi^2\int_0^\infty \mathrm{d}r_1'\int_0^\infty \mathrm{d}R_1'\ \langle r_1R_1|G_1|r_1'R_1'\rangle\frac{r_1'R_1'}{r_1R_1}V_1(r_1') \\
&\quad\times\int_{-1}^{1}\mathrm{d}x'\ \frac{u(r_2',R_2';k)}{r_2'R_2'k}\frac{1}{(4\pi)^{1/2}}\,.
\end{aligned} \tag{3.37}$$

Multiplying both sides of Eq. (3.37) with r_1R_1k gives the final form

$$\begin{aligned}
u(r_1,R_1;k) &= u_b(r_1)\sin(kR_1) + \int_0^\infty \mathrm{d}r_1'\int_0^\infty \mathrm{d}R_1'\ \langle r_1R_1|G_1|r_1'R_1'\rangle r_1'R_1'V_1(r_1')\int_{-1}^{1}\mathrm{d}x'\ \frac{u(r_2',R_2';k)}{r_2'R_2'} \\
&= u_b(r_1)\sin(kR_1) + \int_0^\infty \mathrm{d}r_1'\int_0^\infty \mathrm{d}R_1'\ \langle r_1R_1|G_1|r_1'R_1'\rangle V_1(r_1')Q(r_1',R_1')
\end{aligned} \tag{3.38}$$

with the source term

$$Q(r_1,R_1) := \int_{-1}^{1}\mathrm{d}x\frac{r_1R_1}{r_2R_2}u(r_2,R_2)\,. \tag{3.39}$$

The argument k in the wave functions $u(r_1,R_1;k)$ and $u(r_2,R_2;k)$ is not essential for the following consideration and will be suppressed. We can derive the differential form of the simplified Faddeev equation (3.38) using the channel Hamiltonian $\hat{H}_1 = T_1 + V(r_1)$ in coordinate space representation,

$$\begin{aligned}
\hat{H}_1 &= -\frac{1}{2(m_1+m_2+m_3)}\frac{\mathrm{d}^2}{\mathrm{d}R_{cm}^2} - \frac{1}{2\mu_{23}}\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{1}{2\mu_{1(23)}}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} + V(r_1) \\
&= -\frac{1}{6}\frac{\mathrm{d}^2}{\mathrm{d}R_{cm}^2} - \frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} + V(r_1)\ .
\end{aligned} \tag{3.40}$$

It describes the dynamic of a bound or scattered state between particles 2 and 3 and particle 1 moving freely. With the chosen units the reduced mass $\mu_{1(23)}$ is simply

$$\mu_{1(23)} = \frac{m_1(m_2+m_3)}{m_1+m_2+m_3} = \frac{2}{3}\,. \tag{3.41}$$

The motion of the center of mass is trivial an will be neglected in the following.

Acting with $(E - \hat{H}_1)$ on both sides of Eq. (3.38) gives a partial integrodifferential equation,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} + V(r_1) - E\right]u(r_1, R_1) = \left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} + V(r_1) - E\right][u_b(r_1)\sin(kR_1)]$$
$$+ \int_0^\infty \mathrm{d}r_1' \int_0^\infty \mathrm{d}R_1' \left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} + V(r_1) - E\right]\langle r_1 R_1|G_1|r_1' R_1'\rangle V_1(r_1') \int_{-1}^{1} \mathrm{d}x' \, \frac{r_1' R_1'}{r_2' R_2'} u(r_2', R_2') \,. \tag{3.42}$$

The fact that the incoming state $u_b(r_1)\sin(kR_1)$ is an eigenstate of $\hat{H}_1$ and the identity

$$(E - \hat{H}_1)\langle r_1 R_1|G_1|r_1' R_1'\rangle = (E - \hat{H}_1)\langle r_1 R_1|\frac{1}{E - \hat{H}_1}|r_1' R_1'\rangle = \delta(\mathbf{r}_1 - \mathbf{r}_1')\delta(\mathbf{R}_1 - \mathbf{R}_1') \tag{3.43}$$

lead to the concise expression

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} + V_1(r_1) - E\right]u(r_1, R_1)$$
$$= -\int_0^\infty \mathrm{d}r_1' \int_0^\infty \mathrm{d}R_1' \, \delta(\mathbf{r}_1 - \mathbf{r}_1')\delta(\mathbf{R}_1 - \mathbf{R}_1') V_1(r_1') \int_{-1}^{1} \mathrm{d}x' \, \frac{r_1' R_1'}{r_2' R_2'} u(r_2', R_2') = -V_1(r_1) \int_{-1}^{1} \mathrm{d}x \, \frac{r_1 R_1}{r_2 R_2} u(r_2, R_2) \,, \tag{3.44}$$

with boundary conditions for outgoing scattered waves. After having carried out the integration over both delta-functions, $r_2' \to r_2$ and $R_2' \to R_2$ because r_2 and R_2 are functions of r_1 and R_1 (Eqs. (3.25) and (3.26)).

3.2.1 Asymptotic behavior

We are interested in the asymptotic behavior of $u(r_1, R_1)$ for $R_1 \to \infty$ and $r_1 \to \infty$, which can be deduced from Eq. (3.44) in its asymptotic limit,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} - E\right]u(r_1, R_1) = 0 \,. \tag{3.45}$$

One introduces polar coordinates

$$\begin{aligned} r_1 &= \rho\cos\varphi \,, \\ R_1 &= \sqrt{\frac{3}{4}}\rho\sin\varphi \,. \end{aligned} \tag{3.46}$$

The factor $\sqrt{\frac{3}{4}}$ in the second line of Eq. (3.46) results from the reduced mass, appearing in the Green's function (3.54a). The asymptotic form of $u(\rho,\varphi)$ in the limit $\rho\to\infty$ reads

$$u(\rho,\varphi) \underset{\substack{\rho\to\infty \\ 0<\varphi<\pi/2}}{\backsimeq} \frac{\mathrm{e}^{i\sqrt{E}\rho}}{\rho^{1/2}}\mathrm{A}(\varphi)\,, \tag{3.47}$$

where $\mathrm{A}(\varphi)$ is an unspecified function in φ. This can be verified by transforming the asymptotic Hamiltonian from Eq. (3.45) into polar coordinates (Eq. (3.46)) and let it act onto $u(\rho,\varphi)$ from Eq. (3.47),

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}-\frac{1}{\rho^2}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}-E\right]\left(\frac{\mathrm{e}^{i\sqrt{E}\rho}}{\rho^{1/2}}\mathrm{A}(\varphi)\right)\underset{\rho\to\infty}{\longrightarrow}0\,. \tag{3.48}$$

The detailed calculation is shown in Appendix A.

The convergence of the integral with respect to R_1' in Eq. (3.38), exclusively depends on the source term $Q(r_1,R_1)$ (Eq. (3.39)) as the potential $V(r_1')$ only confines r_1', the distance between particles 2 and 3. So we have to investigate the source term's behavior for $R_1\to\infty$, while assuming a finite range of interaction r_0, limiting r_1' to that value. For that purpose we need the asymptotic form of $u(r_2,R_2)$ given in Eq. (3.47). The transformation of R_2 and r_2 into polar coordinates reads

$$\begin{aligned} r_2 &= \rho\cos\varphi \\ R_2 &= \sqrt{\frac{3}{4}}\rho\sin\varphi. \end{aligned} \tag{3.49}$$

Considering the relation between Jacobi coordinates in Eq. (3.24) we can write (compare Eqs. (3.25)-(3.28))

$$\begin{aligned} r_2(x) =& \sqrt{\frac{1}{4}r_1^2+R_1^2+\mathbf{R}_1\mathbf{r}_1} = \sqrt{\frac{1}{4}r_1^2+R_1^2+R_1r_1x} \\ =& R_1\sqrt{1+\frac{r_1^2}{4R_1^2}+\frac{r_1}{R_1}x} \approx R_1(1+\frac{r_1}{2R_1}x+...) = R_1+\frac{1}{2}r_1x+... \end{aligned} \tag{3.50}$$

and analogously

$$\begin{aligned} R_2(x) &= \sqrt{\frac{9}{16}r_1^2+\frac{1}{4}R_1^2-\frac{3}{4}\mathbf{R}_1\mathbf{r}_1} = \sqrt{\frac{1}{4}R_1^2+\frac{9}{16}r_1^2+\frac{3}{4}R_1r_1x} \\ &= \frac{1}{2}R_1\sqrt{1+\frac{9r_1^2}{4R_1^2}-3\frac{r_1}{R_1}x} \approx \frac{1}{2}R_1(1-\frac{3r_1}{2R_1}x+...) = \frac{1}{2}R_1-\frac{3}{4}r_1x+...\ , \end{aligned} \tag{3.51}$$

where x is the cosine of the angle between $\mathbf{r}_1$ and $\mathbf{R}_1$. The Taylor approximation is valid for $R_1\to\infty$. With the help of Eqs. (3.50) and (3.51) we can determine the angle φ in Eq. (3.49) by keeping only the first terms of the expansions,

$$\tan\varphi = \frac{R_2}{r_2}\sqrt{\frac{4}{3}} \approx \frac{R_1}{2R_1}\sqrt{\frac{4}{3}} = \sqrt{\frac{1}{3}} \Rightarrow \varphi = \arctan\frac{1}{\sqrt{3}} = 30^\circ\,. \tag{3.52}$$

In order to establish the asymptotic form of $Q(r_1,R_1)$ we approximate $R_2(x)$ and $r_2(x)$ by the first term of the expansions in Eqs. (3.50) and (3.51), respectively and use the form (3.47) for $u(r_2,R_2)$. This is valid because for $R_1\to\infty$ it follows from Eq. (3.24) that both, r_2 and R_2 tend towards infinity. Together with the transformation (3.49), we finally obtain,

$$\begin{aligned}
Q(r_1,R_1) &= \int_{-1}^{1}\mathrm{d}x\frac{r_1R_1}{r_2R_2}u(r_2,R_2) \underset{\substack{R_1\to\infty\\ r_1\,\text{fixed}}}{\backsimeq} \int_{-1}^{1}\mathrm{d}x\frac{r_1R_1}{R_1\frac{1}{2}R_1}\frac{\mathrm{e}^{i\sqrt{E}\frac{1}{2}R_1\sqrt{\frac{4}{3}}/\sin 30^\circ}}{\left(\frac{4}{3}\right)^{1/4}\sqrt{\frac{1}{2}R_1\frac{1}{\sin 30^\circ}}}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\\
&= \int_{-1}^{1}\mathrm{d}x\frac{2r_1}{R_1}\frac{\mathrm{e}^{i\sqrt{E}\frac{1}{2}R_1 2\sqrt{\frac{4}{3}}}}{\left(\frac{4}{3}\right)^{1/4}\sqrt{\frac{1}{2}R_1 2}}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right) = \int_{-1}^{1}\mathrm{d}x\;2\left(\frac{3}{4}\right)^{1/4} r_1\frac{\mathrm{e}^{i\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\\
&= 4\left(\frac{3}{4}\right)^{1/4} r_1\frac{\mathrm{e}^{i\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\,.
\end{aligned} \tag{3.53}$$

We find a $R_1^{-3/2}$-dependence in the asymptotic form of $Q(r_1,R_1)$ which assures absolute convergence of the integral over R_1' when calculating $u(r_1,R_1)$ in Eq. (3.56).
The R-matrix approach, we want to establish in Subsections 3.2.2 and 3.2.3, requires the asymptotic form of the solution $u(r_1,R_1)$ of Eq.(3.44), for $R_1\to\infty$ and r_1 fixed and for $r_1\to\infty$ and R_1 fixed, respectively. Each of the two forms can be established by using different representations of the Green's function $G_1=(E-\hat{H}_1)^{-1}$ [6],

$$\begin{aligned}
\langle r_1R_1|G_1|r_1'R_1'\rangle &= u_b(r_1)\left(-\frac{4}{3}\mathrm{e}^{iQR_>}\frac{\sin(QR_<)}{Q}\right)u_b(r_1')\\
&\quad+\frac{2}{\pi}\int_0^\infty\mathrm{d}k\;u_k^{(-)}(r_1)\left(-\frac{4}{3}\mathrm{e}^{iQ_kR_>}\frac{\sin(Q_kR_<)}{Q_k}\right)u_k^{(-)*}(r_1') &\text{(3.54a)}\\
&= \frac{2}{\pi}\int_0^\infty\mathrm{d}K\;\sin(KR_1)\left(-\frac{1}{q_K}u_{q_K}^{(+)}(r_<)w_{q_K}(r_>)\right)\sin(KR_1')\,, &\text{(3.54b)}
\end{aligned}$$

where $R_>=\max(R,R')$, $R_<=\min(R,R')$ and $r_>=\max(r,r')$, $r_<=\min(r,r')$. In Eq. (3.54a) there appears the free Green's function for angular momentum $l=0$ (compare (3.31)) of particle 1 versus the subsystem formed by particles 2 and 3, which is characterized by a complete set of bound-, $u_b(r_1)$, and scattering states $u_k^{(-)}(r_1)$. The second form (3.54b) represents the influence of bound- and scattering states in the subsystem consisting of particles 2 and 3 on the motion of particle 1. The bound- and scattering states $u_{q_K}^{(\pm)}(r)$ and $w_{q_K}(r)$ are normalized as $u_q^{(\pm)}(r)\backsimeq\mathrm{e}^{\pm\mathrm{i}\delta(q)}\sin(qr+\delta(q))$ and $w_q(r)\backsimeq\mathrm{e}^{\mathrm{i}qr}$. The relations between the different wavenumbers occurring in the two representations of G_1 read

$$
\begin{aligned}
E &= -\frac{1}{2\mu_{(23)}}\kappa^2 + \frac{1}{2\mu_{1(23)}}Q^2 = \frac{1}{2\mu_{(23)}}k^2 + \frac{1}{2\mu_{1(23)}}Q_k^2 = \frac{1}{2\mu_{(23)}}q_K^2 + \frac{1}{2\mu_{1(23)}}K^2 \\
E &= E_b + \frac{3}{4}Q^2 = k^2 + \frac{3}{4}Q_k^2 = q_K^2 + \frac{3}{4}K^2 ,
\end{aligned} \tag{3.55}
$$

where we inserted the reduced masses, Eqs. (3.22) and (3.41), in the second line and set $\frac{-\kappa^2}{2\mu_{(23)}} \equiv E_b$. Inserting Eq. (3.54a) into Eq. (3.38) yields the the asymptotic form of $u(r_1, R_1)$ for $R_1 \to \infty$ and r_1 fixed,

$$
\begin{aligned}
u(r_1, R_1) = {} & u_b(r_1)\sin(QR_1) - \frac{4}{3}u_b(r_1)\mathrm{e}^{\mathrm{i}QR_1}\int_0^{R_1} \mathrm{d}R_1' \, \frac{\sin(QR_1')}{Q}\int_0^\infty \mathrm{d}r_1' \; u_b(r_1')V(r_1')Q(r_1', R_1') \\
& - \frac{4}{3}u_b(r_1)\frac{\sin(QR_1)}{Q}\int_{R_1}^\infty \mathrm{d}R_1' \; \mathrm{e}^{\mathrm{i}QR_1'}\int_0^\infty \mathrm{d}r_1' \; u_b(r_1')V(r_1')Q(r_1', R_1') \\
& - \frac{4}{3}\cdot\frac{2}{\pi}\int_0^{\sqrt{E}} \mathrm{d}k \; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_kR_1}\int_0^{R_1} \mathrm{d}R_1' \; \frac{\sin(Q_kR_1')}{Q_k}\int_0^\infty \mathrm{d}r_1' \; u_k^{(-)*}(r_1')V(r_1')Q(r_1', R_1') \\
& - \frac{4}{3}\cdot\frac{2}{\pi}\int_{\sqrt{E}}^\infty \mathrm{d}k \; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_kR_1}\int_0^{R_1} \mathrm{d}R_1' \; \frac{\sin(Q_kR_1')}{Q_k}\int_0^\infty \mathrm{d}r_1' \; u_k^{(-)*}(r_1')V(r_1')Q(r_1', R_1') \\
& - \frac{4}{3}\cdot\frac{2}{\pi}\int_0^\infty \mathrm{d}k \; u_k^{(-)}(r_1)\frac{\sin(Q_kR_1')}{Q_k}\int_{R_1}^\infty \mathrm{d}R_1' \; \mathrm{e}^{\mathrm{i}Q_kR_1}\int_0^\infty \mathrm{d}r_1' \; u_k^{(-)*}(r_1')V(r_1')Q(r_1', R_1') .
\end{aligned} \tag{3.56}
$$

The sixth term on the right hand side of Eq. (3.56) vanishes for $R_1 \to \infty$ because the lower limit of the integral over R_1' then tends to infinity as well as the upper one and the value of the integral becomes zero. The third term of Eq. (3.56) will be treated separately,

$$
\begin{aligned}
H_1(R_1) &= -\frac{4}{3}\int_{R_1}^\infty \mathrm{d}R_1' \; \frac{\sin[Q(R_1 - R_1')]}{Q}\int_0^{r_0} \mathrm{d}r_1' \; r_1' u_b(r_1')V(r_1')Q(r_1', R_1') \\
&\backsimeq -4\left(\frac{3}{4}\right)^{1/4} \mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\frac{1}{E_b}\int_0^{r_0} \mathrm{d}r_1' \; r_1' u_b(r_1')V(r_1') .
\end{aligned} \tag{3.57}
$$

as well as the fifth one,

$$
\begin{aligned}
H_2(r_1,R_1) = &-\frac{4}{3}\cdot\frac{2}{\pi}\int\limits_{\sqrt{E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_kR_1}\int\limits_0^{R_1}\mathrm{d}R_1'\;\frac{\sin(Q_kR_1')}{Q_k}\int\limits_0^{\infty}\mathrm{d}r_1'\; u_k^{(-)*}(r_1')V(r_1')Q(r_1',R_1') \\
&\backsimeq -\frac{8}{\pi}\left(\frac{3}{4}\right)^{1/4}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\int\limits_{\sqrt{E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_1)\frac{1}{k^2} \\
&\times\int\limits_0^{r_0}\mathrm{d}r_1'\; r_1' u_k^{(-)*}(r_1')V(r_1') + O\left(\frac{1}{R_1^2}\right).
\end{aligned}
\tag{3.58}
$$

Due to $E = k^2 + \frac{3}{4}Q_k^2$ it is evident that in the interval $[\sqrt{E};\infty]$ the wavenumber Q_k appears as a complex quantity in $H_2(r_1,R_1)$. Detailed calculations of the integrals over R_1' in Eqs. (3.57) and (3.58) are shown in Appendix B. In both terms we have to insert the asymptotic form (3.53) of $Q(r_1,R_1)$ since $R_1\to\infty$ and thus R_1' becomes sufficiently large in the respective integration intervals, while r_1' is limited by the range r_0 of the potential V.

According to [6] we define

$$
C_b = 4\left(\frac{3}{4}\right)^{1/4}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{1}{E_b}\int\limits_0^{r_0}\mathrm{d}r\; r u_b(r)V(r) \tag{3.59}
$$

and

$$
C(k) = 4\left(\frac{3}{4}\right)^{1/4}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{1}{k^2}\int\limits_0^{r_0}\mathrm{d}r\; r u_k^{(-)*}(r)V(r)\,. \tag{3.60}
$$

and rewrite (3.56) by using the T-amplitudes

$$
T_b = \int\limits_0^{\infty}\mathrm{d}R\int\limits_0^{\infty}\mathrm{d}r\;\frac{\sin(QR)}{Q}u_b(r)V(r)Q(r,R) \tag{3.61}
$$

and

$$
T(k) = \int\limits_0^{\infty}\mathrm{d}R\int\limits_0^{\infty}\mathrm{d}r\;\frac{\sin(Q_kR)}{Q_k}u_k^{(-)*}(r)V(r)Q(r,R) \tag{3.62}
$$

in the following way

$$
\begin{aligned}
u(r_1,R_1) \backsimeq\; & u_b(r_1)\sin(QR_1) - \frac{4}{3}u_b(r_1)\mathrm{e}^{\mathrm{i}QR_1}T_b - \frac{4}{3}\cdot\frac{2}{\pi}\int\limits_0^{\sqrt{E}}\mathrm{d}k\; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_kR_1}T(k) \\
&- \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\left(u_b(r_1)C_b + \frac{2}{\pi}\int\limits_{\sqrt{E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_1)C(k)\right) + O\left(\frac{1}{R_1^2}\right).
\end{aligned}
\tag{3.63}
$$

Eq. (3.63) reveals T_b being the elastic (or rearrangement) scattering amplitude. After having established the asymptotic form of $u(r_1, R_1)$ for $R_1 \to \infty$ and r_0 fixed, we study its asymptotic behavior for R_1 fixed and $r_1 \to \infty$ which is required for the R-matrix formalism. To that end we insert the second form of the Green's function (Eq. (3.54b)) into Eq. (3.38) which gives

$$\begin{aligned} u(r_1, R_1) = &-\frac{2}{\pi} \int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K \ \sin(KR_1) w_{q_K}(r_1) \int_0^{r_1} \mathrm{d}r_1' \ \frac{u_{q_K}^{(+)}(r_1')}{q_K} \int_0^{\infty} \mathrm{d}R_1' \ \sin(KR_1') V(r_1') Q(r_1', R_1') \\ &-\frac{2}{\pi} \int_{\sqrt{\frac{4}{3}E}}^{\infty} \mathrm{d}K \ \sin(KR_1) w_{q_K}(r_1) \int_0^{r_1} \mathrm{d}r_1' \ \frac{u_{q_K}^{(+)}(r_1')}{q_K} \int_0^{\infty} \mathrm{d}R_1' \ \sin(KR_1') V(r_1') Q(r_1', R_1') \\ &-\frac{2}{\pi} \int_0^{\infty} \mathrm{d}K \ \sin(KR_1) u_{q_K}^{(+)}(r_1) \int_{r_1}^{\infty} \mathrm{d}r_1' \ \frac{w_{q_K}(r_1')}{q_K} \int_0^{\infty} \mathrm{d}R_1' \ \sin(KR_1') V(r_1') Q(r_1', R_1') \end{aligned} \tag{3.64}$$

In the limit $r_1 \to \infty$ the lower bound of the r_1'-integral in the last term continuously approaches the upper one, which leads to a vanishing integral and the term can be neglected. The second term is considered to be a correction term and is treated in Appendix B. Using the asymptotic form of $w_q(r)$ from above, $w_q(r) \backsimeq \mathrm{e}^{\mathrm{i}qr}$, one obtains

$$u(r_1, R_1) \backsimeq -\frac{2}{\pi} \int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K \ \sin(KR_1) \mathrm{e}^{\mathrm{i}q_K r_1} \int_0^{\infty} \mathrm{d}r_1' \ \frac{u_{q_K}^{(+)}(r_1')}{q_K} \int_0^{\infty} \mathrm{d}R_1' \ \sin(KR_1') V(r_1') Q(r_1', R_1') + O\left(\frac{1}{r_1^2}\right) . \tag{3.65}$$

Introducing the amplitude $\overline{T}(K)$

$$\overline{T}(K) = \int_0^{\infty} \mathrm{d}R \int_0^{\infty} \mathrm{d}r \ \sin(KR) \frac{u_{q_K}^{(+)}}{q_K} V(r) Q(r, R) \tag{3.66}$$

provides a compact form of $u(r_1, R_1)$, which reads

$$u(r_1, R_1) \backsimeq -\frac{2}{\pi} \int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K \ \sin(KR_1) \mathrm{e}^{\mathrm{i}q_K r_1} \overline{T}(K) + O\left(\frac{1}{r_1^2}\right) . \tag{3.67}$$

Having defined the T-amplitudes, we can establish some relation between $T(k)$

$$T(k) = \int_0^{\infty} \mathrm{d}R \int_0^{\infty} \mathrm{d}r \ \frac{\sin(Q_k R)}{Q_k} u_k^{(-)*}(r) V(r) Q(r, R)$$

and $\overline{T}(K)$, which are similar with respect to their functional form. First, we write $T(k)$ as a function of q_K,

$$T(q_K) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \; \frac{u_{q_K}^{(-)*}(r)}{Q_{q_K}} \sin(Q_{q_K} R) V(r) Q(r,R)\,. \tag{3.68}$$

In order to proceed, we have to clarify the meaning of Q_{q_K}. Therefore we consider the energy-wave number relation, Eq. (3.55), including the equality

$$E = k^2 + \frac{3}{4} Q_k^2 = q_K^2 + \frac{3}{4} K^2 \tag{3.69}$$

from which we can conclude $Q_{q_K} \equiv K$. This can be interpreted as follows: Q_k is the wave number of particle 1 associated to the wave number k from the subsystem of particles 2 and 3 via the energy relation. Similarly Q_{q_K} is related to q_K, and is called, according to Eq. (3.69), K. Thus,

$$T(q_K) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \; \frac{u_{q_K}^{(-)*}(r)}{K} \sin(KR) V(r) Q(r,R)\,. \tag{3.70}$$

Comparing Eq. (3.66) with Eq. (3.70), one finds the relationship,

$$\overline{T}(K) = \frac{K}{q_K} T(q_K)\,. \tag{3.71}$$

In order to provide a relationship between $T(q_k)$ and $T(k)$, we use an argument, valid for the asymptotic area with $r_1 \to \infty$ and R_1 fixed. Latter describes the break-up channel, where particles 2 and 3 move freely with the distance between them tending to infinity. In that case, the bound state wave function completely disappears in both forms of the Green's function G_1 in Eqs. (3.54a) and (3.54b). This allows us to identify $k \hat{=} q_K$ and $Q_k \hat{=} K$. That means we have a one to one correspondence between the wave numbers on each side of Eq. (3.69), not only the sum of the squares, but also the wave numbers themselves become equal. Consequently, in that limit $T(q_k)$ and $T(k)$ will also be equal to each other. Hence, Eq. (3.67) can be rewritten as

$$\begin{aligned} u(r_1, R_1) &\backsimeq -\frac{2}{\pi} \int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K \; \sin(KR_1) \mathrm{e}^{\mathrm{i}q_K r_1} \overline{T}(K) + O\left(\frac{1}{r_1^2}\right) \\ &= -\frac{2}{\pi} \int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K \; \sin(KR_1) \mathrm{e}^{\mathrm{i}q_K r_1} \frac{K}{q_K} T(q_K) + O\left(\frac{1}{r_1^2}\right) \\ &= -\frac{2}{\pi} \int_{\sqrt{E}}^{0} \mathrm{d}q_K \; \left(-\frac{4}{3}\right) \frac{q_K}{K} \sin(KR_1) \mathrm{e}^{\mathrm{i}q_K r_1} \frac{K}{q_K} T(q_K) + O\left(\frac{1}{r_1^2}\right) \\ &= -\frac{8}{3\pi} \int_0^{\sqrt{E}} \mathrm{d}k \; \sin(KR_1) \mathrm{e}^{\mathrm{i}k r_1} T(k) + O\left(\frac{1}{r_1^2}\right)\,. \end{aligned} \tag{3.72}$$

In the second equality we made use of Eq. (3.71). Then the integration variable K was substituted by q_K according to Eq. (3.69). Differentiating Eq. (3.69) with respect to q_K and K yields

$$\begin{aligned} 0 &= 2q_K \mathrm{d}q_K + \frac{3}{4} 2K \mathrm{d}K \\ \mathrm{d}K &= \left(-\frac{4}{3}\right) \frac{q_K}{K} \mathrm{d}q_K \,. \end{aligned} \tag{3.73}$$

In the last equality q_K was replaced by k due to the one to one correspondence of the wave numbers discussed above. Thus we succeeded to express the asymptotic form of $u(r_1, R_1)$ by the three-body on-shell T-matrix elements T_b and $T(k)$ for both cases, $R_1 \to \infty$, r_1 fixed and R_1 fixed, $r_1 \to \infty$. The next step towards an R-matrix formalism is to extract the leading behavior of $u(r_1, R_1)$ in the limit $r_1 \to \infty$ and $R_1 \to \infty$, equivalent to the break-up channel. This is achieved by the method of steepest descent [11] or saddle point method, applied to the integrals in Eqs. (3.63) and (3.72). It is useful to transform both, Jacobi coordinates and momenta, into polar coordinates.

$$\begin{aligned} r_1 &= \rho \cos\varphi \,, & q_K &= \sqrt{E} \cos\alpha \,, \\ R_1 &= \sqrt{\frac{3}{4}} \rho \sin\varphi \,, & K &= \sqrt{\frac{4}{3} E} \sin\alpha \,. \end{aligned} \tag{3.74}$$

Hence, $u(r_1, R_1)$ from Eq. (3.72) becomes

$$I_2 = -\frac{1}{\pi \mathrm{i}} \sqrt{\frac{4}{3} E} \int\limits_{-\pi/2}^{\pi/2} \mathrm{d}\alpha \, \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)} \cos\alpha \, \overline{T} \left(\sqrt{\frac{4}{3} E} \sin\alpha \right) \,. \tag{3.75}$$

A detailed derivation of Eq. (3.75) is provided in Appendix C.

The leading terms of the integral I_2 for the case that ρ tends to infinity will be calculated via the method of steepest descent. The limit $\rho \to \infty$ implies that $r_1 \to \infty$ and $R_1 \to \infty$, equivalent to the asymptotics of the break-up channel. The method of steepest descent allows one to approximate integrals of the type

$$I = \int\limits_{\Gamma} \mathrm{d}z \; g(z) \mathrm{e}^{t h(z)} \,, \tag{3.76}$$

where $t \to \infty$. It extends the idea of Laplace's method [11] to integrals in the complex plane [12]. Cauchy's integral theorem states, that the value of contour integrals is not changed by continuous deformation of the contour unless it contains any singularities of the integrand and the end points remain the same. The contour Γ is deformed in a way that the maximum of $\mathrm{Re}\, g(z)$, characterized by the complex derivative $g'(z) = 0$, becomes a stationary point of $\mathrm{Im}\, h(z)$. We integrate along that path in which we pass the maximum of $\mathrm{Re}\, g(z)$ in the direction of steepest descent. In the vicinity of that point the integral can be approximated by a series expansion [11] and calculated up to the desired order of the parameter t.

In the case of the complex integral I_2, we extend the integration interval into the complex plane and integrate along the contour $\varphi - \alpha = \tau e^{-i\pi/4}$. The saddle point is located at $\alpha = \varphi$. We find that $g = \varphi + \phi\tau$, where $\phi = \exp\left[\frac{1}{2}\pi i - \frac{1}{2} i \arg\left(\frac{d^2}{d\alpha^2} h(\varphi)\right)\right] = \exp\left[\frac{1}{2}\pi i - \frac{1}{2} i \arg(-i)\right] = \exp\left[\frac{1}{2}\pi i - \frac{1}{2} i \frac{3}{2}\pi\right] = \exp\left[i\frac{\pi}{4}\right]$. Then,

$$I_2 \backsimeq \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \sqrt{\frac{4}{3}E} \frac{e^{i\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \left[\cos\varphi\, \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\varphi\right) - \frac{i}{2}\frac{1}{\rho\sqrt{E}}\frac{d^2}{d\varphi^2}\cos\varphi\, \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\varphi\right) + ...\right]. \tag{3.77}$$

These are the leading terms of the integral in Eq. (3.75).

Furthermore it is interesting to investigate how the asymptotic form of $u(r_1, R_1)$ for $r_1 \to \infty$ and R_1 fixed approaches the result from Eq.(3.77). In order to study this question, we transform the momenta appearing in $u(r_1, R_1)$ from Eq. (3.72) into polar coordinates according to the transformation (3.74), while leaving the spatial coordinates unchanged and obtain

$$I_2 = -\frac{2}{\pi}\sqrt{\frac{4}{3}E} \int_0^{\pi/2} d\alpha\, \sin\left(\sqrt{\frac{4}{3}E} R_1 \sin\alpha\right) e^{i r_1 \sqrt{E}\cos\alpha} \cos\alpha\, \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right). \tag{3.78}$$

The leading terms are again extracted by integrating along the path of steepest descent (which we do not carry out explicitly) starting from $\alpha = 0$. With $\overline{T}(0) = 0$ we obtain the result [6]

$$I_2 \backsimeq \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \left(\frac{4}{3}E\right)^{3/2} \frac{e^{i r_1\sqrt{E}}}{(r_1\sqrt{E})^{3/2}} r_1 \left.\frac{d}{dK}\overline{T}(K)\right|_{K=0}. \tag{3.79}$$

Expanding the first term in Eq. (3.77) into a Taylor series at $\varphi = 0$, or equivalently at $K = 0$. Using the expression $K = \sqrt{\frac{4}{3}E}\sin\varphi$ one obtains

$$\begin{aligned}
I_2 &\backsimeq \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \sqrt{\frac{4}{3}E} \frac{e^{i\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \cos\varphi\, \overline{T}(K) \\
&\backsimeq \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \sqrt{\frac{4}{3}E} \frac{e^{i\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \left(1 - \frac{\varphi^2}{2} + ...\right)\left(\overline{T}(0) + \left.\frac{d}{dK}\overline{T}(K)\right|_{K=0}(K-0) + ...\right) \\
&= \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \sqrt{\frac{4}{3}E} \frac{e^{i\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \left(1 - \frac{\varphi^2}{2} + ...\right)\left(0 + \left.\frac{d}{dK}\overline{T}(K)\right|_{K=0}\sqrt{\frac{4}{3}E}\sin\varphi + ...\right) \\
&= \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \frac{4}{3}E \frac{e^{i\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \left(1 - \frac{\varphi^2}{2} + ...\right)\left(\left.\frac{d}{dK}\overline{T}(K)\right|_{K=0}\frac{R_1}{\rho}\sqrt{\frac{4}{3}} + ...\right) \\
&= \sqrt{\frac{2}{\pi}} e^{i\frac{\pi}{4}} \left(\frac{4}{3}E\right)^{3/2} \frac{e^{i r_1\sqrt{E}}}{\left(r_1\sqrt{E}\right)^{3/2}} R_1 \left.\frac{d}{dK}\overline{T}(K)\right|_{K=0}.
\end{aligned} \tag{3.80}$$

In the second last equality we inserted the transformation $R_1 = \sqrt{\frac{4}{3}}\rho\sin\varphi$ from Eq. (3.74). In the last line of Eq. (3.80) we performed the limit $\varphi \to 0$, or equally $K \to 0$, and kept the leading terms only.

Eq. (3.77) exhibits the leading terms of the $u(r_1, R_1)$ in the asymptotic range where $r_1 \to \infty$ and $R_1 \to \infty$. The limit $\varphi \to 0$ implies $r_1 = \rho\cos\varphi \underset{\varphi\to 0}{\longrightarrow} \rho$ and consequently $\rho \to \infty$. In turn this means that $R_1 = \sqrt{\frac{3}{4}}\rho\sin\varphi$ becomes finite. The leading term of of $u(r_1, R_1)$ for $r_1 \to \infty$ and R_1 fixed, however, is presented in Eq. (3.79). Hence, for $\varphi \to 0$ the results of Eq. (3.80) and Eq. (3.79) have to be consistent and so the second derivative term in Eq. (3.77) must vanish in higher order for $\varphi \to 0$.

The leading contributions from the first integral in Eq. (3.63),

$$I_1 = -\frac{8}{3\pi}\int\limits_0^{\sqrt{E}} \mathrm{d}k\; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_k R_1} T(k)\,, \tag{3.81}$$

in the break-up channel, i.e. $r_1 \to \infty$ and $R_1 \to \infty$ can be determined in an analogous way. Applying the following transformation to the integral,

$$\begin{aligned} r_1 &= \rho\sin\beta\,, & k &= \sqrt{E}\sin\vartheta\,, \\ R_1 &= \sqrt{\frac{3}{4}}\rho\cos\beta\,, & Q_k &= \sqrt{\frac{4}{3}}E\cos\vartheta\,, \end{aligned} \tag{3.82}$$

we get

$$I_1 = -\frac{4\sqrt{E}}{3\pi\mathrm{i}}\int\limits_{-\pi/2}^{\pi/2} \mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta)} T\left(\sqrt{E}\sin\vartheta\right)\,. \tag{3.83}$$

A detailed calculation of (3.83) is provided in Appendix D. Again I_1 is approximated by the contribution arising from the saddlepoint $\vartheta = \beta$ in the frame of the method of steepest descent. We set $\vartheta = \beta = \frac{\pi}{2} - \varphi$ and after integration along the path of steepest descent we obtain a result similar to Eq. (3.77), i.e.

$$I_1 \backsimeq \frac{4}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\sqrt{E}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}}\left[\sin\varphi\, T\left(\sqrt{E}\cos\varphi\right) - \frac{\mathrm{i}}{2}\frac{1}{\rho\sqrt{E}}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\sin\varphi\, T\left(\sqrt{E}\cos\varphi\right) + ...\right]\,. \tag{3.84}$$

Inserting the relation $\overline{T}\left(\sqrt{\frac{4}{3}E}\sin\varphi\right) = \sqrt{\frac{4}{3}}\frac{\sin\varphi}{\cos\varphi}T\left(\sqrt{E}\cos\varphi\right)$, which is Eq. (3.71) with transformed momenta according to Eq. (3.74), into Eq. (3.77) yields

$$
\begin{aligned}
I_2 \backsimeq & \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} \sqrt{\frac{4}{3}E} \frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \left[\cos\varphi \sqrt{\frac{4}{3}} \frac{\sin\varphi}{\cos\varphi} T\left(\sqrt{E}\cos\varphi\right) \right. \\
& \left. - \frac{\mathrm{i}}{2} \frac{1}{\rho\sqrt{E}} \frac{\mathrm{d}^2}{\mathrm{d}\varphi^2} \cos\varphi \sqrt{\frac{4}{3}} \frac{\sin\varphi}{\cos\varphi} T\left(\sqrt{E}\cos\varphi\right) + \ldots \right] \\
= & \frac{4}{3}\sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} \sqrt{E} \frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \left[\sin\varphi\, T\left(\sqrt{E}\cos\varphi\right) - \frac{\mathrm{i}}{2} \frac{1}{\rho\sqrt{E}} \frac{\mathrm{d}^2}{\mathrm{d}\varphi^2} \sin\varphi\, T\left(\sqrt{E}\cos\varphi\right) + \ldots \right] .
\end{aligned}
\tag{3.85}
$$

So starting with either the asymptotic form of u where $r_1 \to \infty$ and R_1 fixed or with u where r_1 fixed and $R_1 \to \infty$ leads to the same result for the break-up channel ($r_1 \to \infty$ and $R_1 \to \infty$), which one would also expect. Thus, we can write down the wave function $u(r_1, R_1)$ for the break-up channel,

$$
u(r_1, R_1) \underset{\rho\to\infty}{\backsimeq} \frac{4}{3}\sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}} \sin\varphi\, T\left(\sqrt{E}\cos\varphi\right) . \tag{3.86}
$$

In the break-up channel, the three-particles can no longer interact in the asymptotic region (Fig. 2). Thus, the total energy E is split up into the two relative motions, characterized by the wavenumbers k and Q_k. For every situation there is a defined ratio of r_1/R_1, which determines a specific angle φ_1 in polar coordinates and consequently a specific value for the momentum $k_i = \sqrt{E}\cos\varphi_i$. Because r_2, R_2 and r_3, R_3 are connected with r_1, R_1 by the relations (3.24), $k_2 = \sqrt{E}\cos\varphi_2$ and $k_3 = \sqrt{E}\cos\varphi_3$, get fixed too. The function $T_i(k)$ gives a spectrum of the partition of energy into the two relative motions. A spectrum of the partition of energy into the two relative motions is given by the function $T(k)$. We

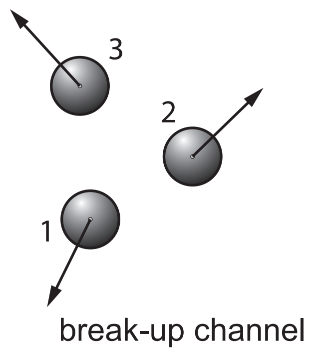

Figure 2: Break-up channel

proceed in calculating the break-up amplitude of one Faddeev component,

$$\begin{aligned}
\psi(r_1, R_1) = \frac{u(r_1,R_1)}{r_1 R_1} &\underset{\rho\to\infty}{\backsimeq} \frac{4}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}}\sin\varphi_1\frac{1}{r_1R_1}T(k_1) \\
&= \frac{4}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}}\sin\varphi_1\sqrt{\frac{4}{3}}\frac{1}{\rho\sin\varphi_1}\frac{1}{\rho\underbrace{\cos\varphi_1}_{=\cos\left(\frac{\pi}{2}-\vartheta_1\right)}}T(k_1) \\
&= \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\frac{T(k_1)}{\sin\vartheta_1} = \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\frac{\sqrt{E}}{k_1}T(k_1) \\
&= \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{3/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\frac{T(k_1)}{k_1}\,.
\end{aligned} \tag{3.87}$$

We used the transformations (3.74) and (3.82) and the saddle point condition $\vartheta = \frac{\pi}{2} - \varphi$, resulting from the integration along the line of steepest descent. Due to the symmetry of the total wave function $\Psi^{(+)}_{break-up}$, the number of Faddeev components reduces from three different ones to one single component, which occurs three times, each depending on one different set of Jacobi coordinates. This has already been discussed in Section 3.2 and means that once we have calculated $\psi(r_1, R_1)$ we have solved the scattering problem for a certain channel and can calculate the scattering wave function according to Eq. (3.1), which is $\Psi^{(+)} = \psi(r_1, R_1) + \psi(r_2, R_2) + \psi(r_3, R_3)$. For the break-up channel we coherently sum up the leading asymptotic parts of the Faddeev component ψ in the limit $r_i \to \infty$ and $R_i \to \infty$ with $i = 1, 2, 3$ (Eq. (3.87)) and obtain (ρ depends on r_i)

$$\Psi^{(+)}_{break-up} = \sum_{i=1}^{3}\psi(r_i,R_i) \underset{\substack{r_i\to\infty\\R_i\to\infty}}{\backsimeq} \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{3/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\left[\frac{T(k_1)}{k_1}+\frac{T(k_2)}{k_2}+\frac{T(k_3)}{k_3}\right]. \tag{3.88}$$

The magnitude ρ is defined according to (3.46) and depends on r_i and R_i in the following way

$$\begin{aligned}
r_i &= \rho\cos\varphi_i\,, \\
R_i &= \sqrt{\frac{3}{4}}\rho\sin\varphi_i\,.
\end{aligned} \tag{3.89}$$

3.2.2 Towards R-matrix theory - interior region and basis states

The key feature of R-matrix theory [13] is the division of the configuration space into two parts: an interior region and an exterior region with the borderlines

$$\begin{aligned}
C_1:\ R = A \quad &\text{and} \quad 0 \le r \le a \\
C_2:\ r = a \quad &\text{and} \quad 0 \le R \le A
\end{aligned} \tag{3.90}$$

between them. Graphically we get a two-dimensional rectangular area for the interior region, bounded by the lines C_1 and C_2 (Fig 3). The Schrödinger equation is solved separately in the interior and exterior region which are connected at the borderlines by suitable boundary conditions following in the next subsection 3.2.3.

The set of all points with $r \geq 0$ and $R \geq 0$ that are located inside that area is called D and we choose $r_1, R_1 \in D$. Moreover we require the second set of Jacobi coordinates (r_2, R_2) being located

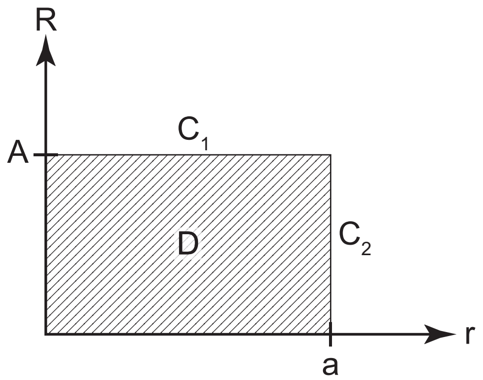

Figure 3: Illustration of the interior region D with boundary lines C_1 and C_2.

in D as well. The potential $V(r_1)$ occurs on the right hand side of Eq. (3.44) due to its finite range r_0 confines the maximum magnitude of r_1 to that value. Outgoing from the relations between Jacobi coordinates (3.24) and using the upper bound approximation for the magnitudes r_2 and R_2,

$$|a\mathbf{r}_1 \pm b\mathbf{R}_1| = \sqrt{(ar_1)^2 \pm 2ab(\mathbf{r}_1 \cdot \mathbf{R}_1) + (bR_1)^2} \approx \sqrt{(ar_1)^2 + 2abr_1R_1 + (bR_1)^2} = ar_1 + bR_1\,, \quad (3.91)$$

the requirement $r_2, R_2 \in D$, i.e. $r_{2_{max}} \leq a$ and $R_{2_{max}} \leq A$, leads to

$$\begin{aligned} &\text{a) } \mathbf{r}_2 = -\frac{1}{2}\mathbf{r}_1 - \mathbf{R}_1 \quad \underset{r_2\ in\ D}{\longrightarrow} \quad \frac{1}{2}r_0 + A \leq a \\ &\text{b) } \mathbf{R}_2 = \frac{3}{4}\mathbf{r}_1 - \frac{1}{2}\mathbf{R}_1 \quad \underset{R_2\ in\ D}{\longrightarrow} \quad \frac{3}{4}r_0 + \frac{1}{2}A \leq A\,. \end{aligned} \quad (3.92)$$

Expressing A explicitly from relation b) and inserting it into relation a) we get (with $\delta > 0$)

$$\begin{aligned} &\text{b) } A \geq \frac{3}{2}r_0 \;\Rightarrow\; A = \frac{3}{2}r_0 + \delta \\ &\text{a) } \frac{3}{2}r_0 + \frac{1}{2}r_0 \leq a \Rightarrow a \geq 2r_0 \Rightarrow a = 2r_0 + \delta\,. \end{aligned} \quad (3.93)$$

Thus, by confining r_2, R_2 to D the boundary parameters a and A can be expressed by the range of the potential r_0 and a parameter $\delta > 0$. Latter can be chosen such that the asymptotic forms of u, Eq. (3.63) and Eq.(3.72), are valid on the lines C_1 and C_2. In the interior region a complete set of basis states $\varphi_\mu(r, R)$ is introduced, which fulfill the equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R^2} - E_\mu\right]\varphi_\mu(r, R) = 0\,. \quad (3.94)$$

with the boundary conditions

$$\varphi_\mu(0,R) = \varphi_\mu(r,0) = \left.\frac{\partial\varphi_\mu(r,R)}{\partial r}\right|_{r=a} = \left.\frac{\partial\varphi_\mu(r,R)}{\partial R}\right|_{R=A} = 0\,. \tag{3.95}$$

Moreover, these states can be chosen real and should fulfill the orthonormalization condition

$$\iint_D \mathrm{d}r\,\mathrm{d}R\;\varphi_\mu(r,R)\varphi_{\mu'}(r,R) = \delta_{\mu\mu'}\,. \tag{3.96}$$

We choose the introduced basis states $\varphi_\mu(r,R)$ as product states

$$\varphi_\mu(r,R) = X_{\mu_1}(r)Y_{\mu_2}(R)\,, \tag{3.97}$$

where the functions $X_{\mu_1}(r)$ and $Y_{\mu_2}(R)$ are solutions to the equations

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) - \epsilon_{\mu_1}\right] X_{\mu_1}(r) = 0 \tag{3.98}$$

and

$$\left[-\frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \epsilon_{\mu_2}\right] Y_{\mu_2}(R) = 0\,. \tag{3.99}$$

The total energy E_μ is split into the energy of the two relative motions, ϵ_{μ_1} (particle 2 relative to particle 3) and ϵ_{μ_2} (particle 1 relative to particle 2 and 3). It is advantageous, to order the set $\mu = \mu_1, \mu_2$ in that way that the total energy $E_\mu = \epsilon_{\mu_1} + \epsilon_{\mu_2}$ is approximately constant [6].

Hence, in the interior region the Faddeev amplitude u can be expanded as

$$u(r_i,R_i) = \sum_\mu c_\mu \varphi_\mu(r_i,R_i)\,, \tag{3.100}$$

with

$$c_\mu = \iint_D \mathrm{d}r\,\mathrm{d}R\;\varphi_\mu(r,R)u(r,R)\,. \tag{3.101}$$

Eq. (3.101) results from integrating both sides of Eq. (3.100) over the region D and using the orthonormalization condition, Eq. (3.96).

3.2.3 Equations for three-body R-matrix theory

In this section we want to establish a set of equations in the frame of three-body R-matrix theory, that allow us to calculate the coefficients c_μ and thus the wave functions in the interior and the three-body on-shell T-matrix elements T_b and T_k, which determine the experimentally accessible cross section (see Subsection 3.2.4). We multiply Eq. (3.44) from the left by $\varphi_\mu(r_1, R_1)$,

$$\varphi_\mu(r_1, R_1)\left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} + V(r_1) - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} - E\right] u(r_1, R_1) = -\varphi_\mu(r_1, R_1)V(r_1)\int\limits_{-1}^{1} \mathrm{d}x\; \frac{r_1 R_1}{r_2 R_2} u(r_2, R_2)\,. \tag{3.102}$$

For clarity we do not explicitly write down the dependencies of u and φ_μ in their derivatives, i.e. $u \equiv u(r, R)$ and $\varphi_\mu \equiv \varphi_\mu(r, R)$. We perform the integration of Eq. (3.102) over the domain D

$$\begin{aligned} &\iint_D \mathrm{d}r\,\mathrm{d}R\;\varphi_\mu(r_1, R_1)\left[-\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} + V(r_1) - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R_1^2} - E\right] u(r_1, R_1) \\ &= -\iint_D \mathrm{d}r\,\mathrm{d}R\;\varphi_\mu(r_1, R_1)V(r_1)\int\limits_{-1}^{1} \mathrm{d}x\; \frac{r_1 R_1}{r_2 R_2} u(r_2, R_2)\,. \end{aligned} \tag{3.103}$$

After some manipulations and the calculation of the various integrals, which can be found in Appendix E, one finally arrives at

$$\begin{aligned} &(E_\mu - E)c_\mu - \frac{3}{4}\int\limits_0^a \mathrm{d}r\;\varphi_\mu(r, A)\left.\frac{\mathrm{d}u}{\mathrm{d}R}\right|_{R=A} - \int\limits_0^A \mathrm{d}R\;\varphi_\mu(a, R)\left.\frac{\mathrm{d}u}{\mathrm{d}r}\right|_{r=a} \\ &= -\iint_D \mathrm{d}r_1\mathrm{d}R_1\;\varphi_\mu(r_1, R_1)V(r_1)\int\limits_{-1}^{1} \mathrm{d}x\; \frac{r_1 R_1}{r_2 R_2} u(r_2, R_2)\,. \end{aligned} \tag{3.104}$$

The right hand side of (3.104) can be further treated

$$\begin{aligned} &-\iint_D \mathrm{d}r_1\mathrm{d}R_1\;\varphi_\mu(r_1, R_1)V(r_1)\int\limits_{-1}^{1} \mathrm{d}x\; \frac{r_1 R_1}{r_2 R_2} u(r_2, R_2) \\ &= -\iint_D \mathrm{d}r_1\mathrm{d}R_1\;\varphi_\mu(r_1, R_1)V(r_1)\int\limits_{-1}^{1} \mathrm{d}x\; \frac{r_1 R_1}{r_2 R_2}\sum_{\mu'} c_{\mu'}\varphi_{\mu'}(r_2, R_2)\,. \end{aligned} \tag{3.105}$$

Because the variables r_2 and R_2 are confined to D which is ensured by the choice of the values (3.93) for the parameters A and a, we can expand $u(r_2, R_2)$ in the source term. After introducing the matrix element

$$V_{\mu\mu'} = \iint_D \mathrm{d}r_1\mathrm{d}R_1\;\varphi_\mu(r_1, R_1)V(r_1)\int\limits_{-1}^{1} \mathrm{d}x\; \frac{r_1 R_1}{r_2 R_2}\varphi_{\mu'}(r_2, R_2)\,, \tag{3.106}$$

Eq. (3.103) in its final form becomes

$$\frac{3}{4}\int\limits_0^a \mathrm{d}r\ \varphi_\mu(r,A)\ \frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} + \int\limits_0^A \mathrm{d}R\ \varphi_\mu(a,R)\ \frac{\mathrm{d}u}{\mathrm{d}r}\bigg|_{r=a} = (E_\mu - E)c_\mu + \sum_{\mu'} V_{\mu\mu'}c_{\mu'}\,. \tag{3.107}$$

Two asymptotic forms of the wave function u have already been established in Eqs. (3.63) and (3.72) and are now inserted for u on the borderlines C_1 and C_2 in Eq. (3.107). This yields

$$\begin{aligned}
&\frac{3}{4}\int\limits_0^a \mathrm{d}r\ \varphi_\mu(r,A)u_b(r)Q\cos(QA) - \frac{3}{4}\frac{4}{3}\int\limits_0^a \mathrm{d}r\ \varphi_\mu(r,A)u_b(r)\mathrm{i}Q\mathrm{e}^{\mathrm{i}QA}T_b \\
&- \frac{3}{4}\frac{4}{3}\frac{2}{\pi}\int\limits_0^a \mathrm{d}r\ \varphi_\mu(r,A)\int\limits_0^{\sqrt{E}} \mathrm{d}k\ u_k^{(-)}(r)\mathrm{i}Q_k\mathrm{e}^{\mathrm{i}Q_kA}T(k) - \frac{3}{4}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}A}}{A^{3/2}}\mathrm{i}\sqrt{\frac{4}{3}E}\int\limits_0^a \mathrm{d}r\ \varphi_\mu(r,A)u_b(r)C_b \\
&- \frac{3}{4}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}A}}{A^{3/2}}\mathrm{i}\sqrt{\frac{4}{3}E}\frac{2}{\pi}\int\limits_0^a \mathrm{d}r\ \varphi_\mu(r,A)\int\limits_0^\infty \mathrm{d}k\ u_k^{(-)}(r)C(k) \\
&- \frac{2}{\pi}\frac{4}{3}\int\limits_0^A \mathrm{d}R\ \varphi_\mu(a,R)\int\limits_0^{\sqrt{E}} \mathrm{d}k\ \sin(Q_kR)\mathrm{i}k\mathrm{e}^{\mathrm{i}ka}T(k) \\
&= (E_\mu - E)c_\mu + \sum_{\mu'} V_{\mu\mu'}c_{\mu'}\,,
\end{aligned} \tag{3.108}$$

where we neglected terms $\sim R^{-\alpha}$ with $\alpha > \frac{3}{2}$. Correction terms of the order $O(1/r^2)$ and $O(1/R^2)$ occurring in the asymptotic forms of u are ignored either. In order to set the numbers C_b and $C(k)$ into relation with the T-amplitudes we compare Eqs. (3.86) and (3.47) and conclude that

$$A(\varphi) = \frac{4}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\sin\varphi\, T(\sqrt{E}\cos\varphi) \tag{3.109}$$

or specifically

$$A\left(\arctan\frac{1}{\sqrt{3}}\right) = \frac{2}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}T\left(\sqrt{\tfrac{3}{4}E}\right)\,. \tag{3.110}$$

Thus,

$$C_b = \left(\frac{3}{4}\right)^{1/4}\frac{8}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}T\left(\sqrt{\tfrac{3}{4}E}\right)\frac{1}{E_b}\int\limits_0^{r_0} \mathrm{d}r\ ru_b(r)V(r) \tag{3.111}$$

and

$$C(k) = \left(\frac{3}{4}\right)^{1/4}\frac{8}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}T\left(\sqrt{\tfrac{3}{4}E}\right)\frac{1}{k^2}\int\limits_0^{r_0} \mathrm{d}r\ ru_k^{(-)*}(r)V(r)\,. \tag{3.112}$$

For reasons of clarity we introduce the following abbreviations,

$$
\begin{aligned}
M_{\mu b} &= \int_0^a \mathrm{d}r\ \varphi_\mu(r,A) u_b(r) \\
M_{\mu k}^{(-)} &= \int_0^a \mathrm{d}r\ \varphi_\mu(r,A) u_k^{(-)}(r) \\
M_{\mu Q} &= \int_0^A \mathrm{d}R\ \varphi_\mu(a,R)\sin(QR)\,.
\end{aligned}
\tag{3.113}
$$

Then we obtain the final form of Eq. (3.108),

$$
\begin{aligned}
&(E_\mu - E)c_\mu + \sum_{\mu'} V_{\mu\mu'} c_{\mu'} = \frac{3}{4} Q M_{\mu b}\cos(QA) - \mathrm{i} Q M_{\mu b} \mathrm{e}^{\mathrm{i}QA} T_b - \frac{2}{\pi}\int_0^{\sqrt{E}} \mathrm{d}k\ \mathrm{i}Q_k M_{\mu k}^{(-)} \mathrm{e}^{\mathrm{i}Q_k A} T(k) \\
&- \frac{3}{4}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}A}}{A^{3/2}} \mathrm{i}\sqrt{\frac{4}{3}E}\left(\frac{3}{4}\right)^{1/4} \frac{8}{3}\sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} T\left(\sqrt{\tfrac{3}{4}E}\right) M_{\mu b} \frac{1}{E_b}\int_0^{r_0} \mathrm{d}r\ r u_b(r) V(r) \\
&- \frac{3}{4}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}A}}{A^{3/2}} \mathrm{i}\sqrt{\frac{4}{3}E}\frac{2}{\pi}\left(\frac{3}{4}\right)^{1/4} \frac{8}{3}\sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} T\left(\sqrt{\tfrac{3}{4}E}\right) \int_0^\infty \mathrm{d}k\ M_{\mu k}^{(-)} \frac{1}{k^2}\int_0^{r_0} \mathrm{d}r\ r u_k^{(-)*}(r) V(r) \\
&- \frac{2}{\pi}\frac{4}{3}\int_0^{\sqrt{E}} \mathrm{d}k\ \mathrm{i}k M_{\mu Q_k} \mathrm{e}^{\mathrm{i}ka} T(k) \\
&= \frac{3}{4} Q M_{\mu b}\cos(QA) - \mathrm{i} Q M_{\mu b} \mathrm{e}^{\mathrm{i}QA} T_b - \frac{2}{\pi}\int_0^{\sqrt{E}} \mathrm{d}k\ \left[\mathrm{i}Q_k M_{\mu k}^{(-)} \mathrm{e}^{\mathrm{i}Q_k A} + \mathrm{i}\frac{4}{3} k M_{\mu Q_k} \mathrm{e}^{\mathrm{i}ka}\right] T(k) \\
&- N(E)\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}A}}{A^{3/2}} T\left(\sqrt{\tfrac{3}{4}E}\right)\left[M_{\mu b}\frac{1}{E_b}\int_0^{r_0} \mathrm{d}r\ r u_b(r) V(r) + \frac{2}{\pi}\int_0^\infty \mathrm{d}k\ M_{\mu k}^{(-)}\frac{1}{k^2}\int_0^{r_0} \mathrm{d}r\ r u_k^{(-)*}(r) V(r)\right],
\end{aligned}
\tag{3.114}
$$

with

$$
N(E) = \left(\frac{3}{4}E\right)^{3/4} \frac{8}{3}\sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\,. \tag{3.115}
$$

In analogy to two-particle scattering we define the three-particle R-matrix according to

$$
R_{\mu\mu'}(E) \equiv \delta_{\mu\mu'}(E_\mu - E) + V_{\mu\mu'}\,. \tag{3.116}
$$

form since $V_{\mu\mu'}$ is defined as Considering the definition

$$V_{\mu\mu'} = \iint_D \mathrm{d}r_1 \mathrm{d}R_1 \, \varphi_\mu(r_1, R_1) V(r_1) \int_{-1}^{1} \mathrm{d}x \, \frac{r_1 R_1}{r_2 R_2} \varphi_{\mu'}(r_2, R_2)$$

from above, one realizes $R_{\mu\mu'}(E)$ to be the matrix representation the Faddeev equations inside the region D.

Eq. (3.114) is the first equation for the R-matrix formalism and connects the expansion coefficients of the interior wave functions, c_μ, with the elements of the T-matrix. Further equations follow by matching the interior and exterior form of u at the boundary lines C_1 and C_2, respectively. We therefore reduce u to its flux conserving terms and ignore terms $\sim 1/R^{3/2}$ and the correction terms of higher order. Furthermore we set $u_b(a) \approx 0$ because the binding state wave function is spatially located and nearly vanishes at the boarder line C_2. This assumption was already made when we derived the form (3.86) of u from Eq. (3.63) for $\rho \to \infty$,

$$u(r_1, R_1) \simeq -\frac{8}{3\pi} \int_0^{\sqrt{E}} \mathrm{d}k \, u_k^{(-)}(r_1) \mathrm{e}^{\mathrm{i}Q_k R_1} T(k) (+...) \underset{\rho\to\infty}{\simeq} \frac{4}{3}\sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}} \sin\varphi \, T\left(\sqrt{E}\cos\varphi\right) \tag{3.117}$$

We neglected the terms containing the binding wave function $u_b(r)$ in Eq. (3.63) before extracting the leading terms via the method of steepest descent and called the new integral I_1 (see Appendix D). Thus, we may conclude that $\int_0^a \mathrm{d}r \, u_b(r) u_k^{(-)}(r) \approx 0$ on the line C_1. Hence, projecting Eq. (3.63) onto $u_b(r)$ and making use of $u_b^*(r) = u_b(r)$ (the binding wave function is real) yields

$$\begin{aligned} \int_0^a \mathrm{d}r \, u_b(r) \sum_\mu c_\mu \varphi_\mu(r, A) \simeq & \underbrace{\int_0^a \mathrm{d}r \, |u_b(r)|^2}_{=1} \sin(QA) - \frac{4}{3} \underbrace{\int_0^a \mathrm{d}r \, |u_b(r)|^2}_{=1} \mathrm{e}^{\mathrm{i}QA} T_b \\ & - \frac{8}{3\pi} \int_0^{\sqrt{E}} \mathrm{d}k \underbrace{\int_0^a \mathrm{d}r \, u_b(r) u_k^{(-)}(r)}_{\approx 0} \mathrm{e}^{\mathrm{i}Q_k A} T(k) \,. \end{aligned} \tag{3.118}$$

Again, using the abbreviations from Eq. (3.113), we finally get

$$\sum_\mu M_{\mu b} c_\mu \simeq \sin(QA) - \frac{4}{3} \mathrm{e}^{\mathrm{i}QA} T_b \,. \tag{3.119}$$

The crucial point is the expansion of $u(r_1, R_1)$ into basis states φ_μ on the left hand side of Eq. (3.118), which is only valid *inside* the region D. On the right hand side, we have the asymptotic form of u *outside* the region D. Both are set equal on the line C_1, which provides another equation in R-matrix formalism. A similar relation for the break-up amplitude $T(k)$ cannot be established via projection on the scattering states $u_k^{(-)}(r)$, because they are not mutually orthogonal on the finite interval $0 \leq r \leq a$. However, we can use the asymptotic form of u in Eq. (3.63),

$$u(r_1, R_1) \underset{R_1\to\infty}{\backsimeq} u_b(r_1)\sin(QR_1) - \frac{4}{3}u_b(r_1)\mathrm{e}^{\mathrm{i}QR_1}T_b - \frac{4}{3}\cdot\frac{2}{\pi}\int_0^{\sqrt{E}} \mathrm{d}k\; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_kR_1}T(k)$$

with the asymptotic expansion (3.86) of the k-integral, outlined in Eq. (3.117)

$$u(r_1, R_1) \underset{\rho\to\infty}{\backsimeq} \frac{4}{3}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}}\sin\varphi\, T\left(\sqrt{E}\cos\varphi\right)$$

to interrelate the expansion coefficients c_μ with the T-matrix elements $T(k)$. When matching the wave function u *inside* D with u *outside* D on the line C_1, we obtain a further relation,

$$\sum_\mu c_\mu\varphi_\mu(r, A) - u_b(r)\left[\sin(QA) - \frac{4}{3}\mathrm{e}^{\mathrm{i}QA}T_b\right] \backsimeq \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho_A\sqrt{E}}}{\rho_A^{1/2}}\frac{A}{\rho_A}\,T\left(\sqrt{E}\frac{r}{\rho_A}\right), \tag{3.120}$$

with $\rho_A = \sqrt{r^2 + \frac{4}{3}A^2}$ and $\sin\varphi|_{C_1} = \sqrt{\frac{4}{3}}\frac{A}{\rho_A}$. On the line C_2 one gets in the same manner,

$$\begin{aligned}\sum_\mu c_\mu\varphi_\mu(a, R) &\backsimeq u_b(a)\left[\sin(QR) - \mathrm{e}^{\mathrm{i}QR}T_b\right] + \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho_a\sqrt{E}}}{\rho_a^{1/2}}\frac{R}{\rho_a}\,T\left(\sqrt{E}\frac{a}{\rho_a}\right)\\ &\backsimeq \left(\frac{4}{3}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho_a\sqrt{E}}}{\rho_a^{1/2}}\frac{R}{\rho_a}\,T\left(\sqrt{E}\frac{a}{\rho_a}\right),\end{aligned} \tag{3.121}$$

with $\rho_a = \sqrt{a^2 + \frac{4}{3}R^2}$ and $u_b(a) \approx 0$.
We have derived a set of four equations for the determination of c_μ and the on-shell T-matrix elements,

$$
\begin{aligned}
&1)(E_\mu - E)c_\mu + \sum_{\mu'} V_{\mu\mu'} c_{\mu'} \\
&= \frac{3}{4} Q M_{\mu b} \cos(QA) - \mathrm{i} Q M_{\mu b} \mathrm{e}^{\mathrm{i}QA} T_b - \frac{2}{\pi} \int\limits_0^{\sqrt{E}} \mathrm{d}k \, \left[\mathrm{i} Q_k M_{\mu k}^{(-)} \mathrm{e}^{\mathrm{i}Q_k A} + \mathrm{i}\frac{4}{3} k M_{\mu Q_k} \mathrm{e}^{\mathrm{i}ka} \right] T(k) \\
&- N(E) \frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}A}}{A^{3/2}} T\left(\sqrt{\tfrac{3}{4}E}\right) \left[M_{\mu b} \frac{1}{E_b} \int\limits_0^{r_0} \mathrm{d}r \, r u_b(r) V(r) + \frac{2}{\pi} \int\limits_{\sqrt{E}}^{\infty} \mathrm{d}k \, M_{\mu k}^{(-)} \frac{1}{k^2} \int\limits_0^{r_0} \mathrm{d}r \, r u_k^{(-)*}(r) V(r) \right] \\
&2) \sum_\mu M_{\mu b} c_\mu \backsimeq \sin(QA) - \frac{4}{3} \mathrm{e}^{\mathrm{i}QA} T_b \\
&3) \sum_\mu c_\mu \varphi_\mu(r, A) - u_b(r) \left[\sin(QA) - \mathrm{e}^{\mathrm{i}QA} T_b \right] \backsimeq \left(\frac{4}{3}\right)^{3/2} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho_A \sqrt{E}}}{\rho_A^{1/2}} \frac{A}{\rho_A} \, T\left(\sqrt{E} \frac{r}{\rho_A}\right) \\
&4) \sum_\mu c_\mu \varphi_\mu(a, R) \backsimeq \left(\frac{4}{3}\right)^{3/2} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho_a \sqrt{E}}}{\rho_a^{1/2}} \frac{R}{\rho_a} \, T\left(\sqrt{E} \frac{a}{\rho_a}\right) .
\end{aligned}
\tag{3.122}
$$

The solutions will be the expansion coefficients c_μ and the three-body on-shell T-matrix elements T_b and $T(k)$, which determine the interior wave function as well as the cross section. Numerical methods will be presented in the near future. In the energy region below the break-up threshold $E = 0$, the set of equations simplifies essentially, as the break-up part of u, the amplitude $T(k)$ becomes exponentially small at the boarder lines C_1 and C_2 and can be neglected there. Then, one has to calculate c_μ and T_b only, which are determined by 1) and 2) in the set of equations above. Below all thresholds where no reactions take place any more, the binding energies of the system are given by the eigenvalues of $R_{\mu\mu'}(E)$.

3.2.4 From the T-matrix elements to the cross section

The T-matrix elements play an important role in scattering theory, as they are needed for the calculation of the cross section [9],

$$
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (2\pi)^4 m \left| T_{q_f q} \right|^2 = (2\pi)^4 m \left| \langle \psi_{q_f}^0 | V | \Psi_q^{(+)} \rangle \right|^2 , \tag{3.123}
$$

with $E_q = E_{q_f}$ for the on-shell T-matrix elements. Here, m is the mass of the projectile and V is the scattering potential. $\Psi_q^{(+)}$ is the outgoing scattering state, the physical solution of the scattering problem. It is generated from a momentum eigenstate ψ_q^0 by the definition [9]

$$
|\Psi_q^{(+)}\rangle = \lim_{\epsilon \to 0} \frac{\mathrm{i}\epsilon}{E_q + \mathrm{i}\epsilon - \hat{H}} |\psi_q^0\rangle \tag{3.124}
$$

and is the solution of the stationary Schrödinger equation

$$(\hat{H} - E_q)\Psi_q^{(+)} = 0\,, \tag{3.125}$$

with $\hat{H} = \hat{H}_0 + V$. The final state $\psi^0_{q_f}$ is characterized by the wavenumber q_f. It is an eigenstate of $\hat{H}_0$ as well as ψ^0_q .

The definition for the T-matrix elements, given in Eq.(3.123), is valid in two-particle scattering theory. The three-body transition amplitude between channel α and β is defined as

$$T_{\beta\alpha} = \langle\phi_\beta|V^\beta|\Psi_\alpha^{(+)}\rangle\,. \tag{3.126}$$

The channel potential

$$V^\beta = V_\alpha + V_\gamma + V_4, \qquad \alpha \neq \beta \neq \gamma\,,$$

is defined according to Section 2, but using capital letters instead of small ones. The break-up channel conveniently carries the index 0 with the corresponding potential $V_0 = 0$ and thus $V^0 = V_1 + V_2 + V_3 + (V_4)$.

The T-amplitudes T_b and $T(k)$, which were derived for channel 1 in Section 3.2.1 obey exactly the definition given in Eq. (3.126). With $\phi_1 = j_0(QR_1)\varphi_b(r_1)\,, \phi_k = kj_0(kr_1)j_0(Q_kR_1),\ \varphi_b(r) = \dfrac{u_b(r)}{r}$ we switch to the abstract vector notation in configuration space and rewrite

$$T_b = \int\limits_0^\infty \mathrm{d}R \int\limits_0^\infty \mathrm{d}r\ \frac{\sin(QR)}{Q} u_b(r)V(r)Q(r,R)$$

as

$$T_b = \langle\phi_1|V_1|\psi_2 + \psi_3\rangle = \langle\phi_1|V_1G_0(V_2 + V_3)|\Psi^{(+)}\rangle = \langle\phi_1|V_2 + V_3|\Psi^{(+)}\rangle\,. \tag{3.127}$$

This expression is valid for distinguishable particles because for the source term Q we inserted the sum $\psi_2 + \psi_3$, which simplifies to ψ_1 in the case of identical particles. In the first equality we inserted the definition of the Faddeev components

$$|\psi_i\rangle = G_0V_i|\Psi^{(+)}\rangle$$

and in the second equality we made use of the relation

$$G_0V_\beta|\phi_\beta\rangle = |\phi_\beta\rangle\,. \tag{3.128}$$

To show its validity we multiply both sides of Eq. (3.128) by G_0^{-1} from the left side which leads to

$$\begin{aligned} G_0^{-1}G_0V_\beta|\phi_\beta\rangle &= G_0^{-1}|\phi_\beta\rangle \\ V_\beta|\phi_\beta\rangle &= (E-\hat{H}_0)|\phi_\beta\rangle \\ V_\beta|\phi_\beta\rangle &= (E-E_0)|\phi_\beta\rangle \\ V_\beta|\phi_\beta\rangle &= V_\beta|\phi_\beta\rangle\,. \end{aligned}$$

Here, $\hat{H}_\beta = \hat{H}_0 + V_\beta$ with the eigenstate $|\phi_\beta\rangle$, $\hat{H}_\beta|\phi_\beta\rangle = E|\phi_\beta\rangle$, with $E = E_0 + V_\beta$. From the result of Eq. (3.127) we learn that the total asymptotic behavior of the wave function in channel 1 is contained in the Faddeev component $|\psi_1\rangle$. This can be seen by calculating the amplitude T_b for transitions into channel 1 ($\hat{=}\,\alpha$) according to Eq. (3.126) (β and γ denote channel 2 and 3)

$$T_b = \langle\phi_\alpha|V^\alpha|\Psi^{(+)}\rangle = \langle\phi_\alpha|V_\beta + V_\gamma|\Psi^{(+)}\rangle\,. \tag{3.129}$$

This yields exactly the same result as obtained in Eq. (3.127), where we inserted the functional form of T_b corresponding to $|\psi_1\rangle$.

Next, we want to show that the break-up amplitude

$$T(k) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r\ \frac{\sin(Q_kR)}{Q_k} u_k^{(-)*}(r)V(r)Q(r,R)$$

is in agreement with the definition (3.126). In order to demonstrate this statement we switch to the vector notation and obtain for the first Faddeev component

$$T(k) = \langle\phi_k^{(-)}|V_1|\psi_2 + \psi_3\rangle\,. \tag{3.130}$$

The scattering state $|\phi_k^{(+)}\rangle$ is a solution of the Lippmann-Schwinger equation

$$|\phi_k^{(+)}\rangle = |\phi_k\rangle + G_0V_1|\phi_k^{(+)} = |\phi_k\rangle + \lim_{\epsilon\to 0}\frac{1}{E + \mathrm{i}\epsilon - \hat{H}_0}V_1|\phi_k^{(+)}\rangle\,, \tag{3.131}$$

where $|\phi_k\rangle$ is the solution of the homogenous equation $(E-\hat{H}_0)|\phi_k\rangle = 0$ and $(E-\hat{H}_0)|\phi_k^{(+)}\rangle = V_1|\phi_k^{(+)}\rangle$. The total solution of the scattering problem

$$\hat{H}_1|\phi_k^{(+)}\rangle = E|\phi_k^{(+)}\rangle \tag{3.132}$$

is given by the Lippmann-Schwinger equation (3.131). It can be represented as

$$|\phi_k^{(+)}\rangle = |\phi_k\rangle + G_1V_1|\phi_k\rangle\,, \tag{3.133}$$

which follows from the formal solution of the Lippmann-Schwinger equation

$$
\begin{aligned}
|\phi_k^{(+)}\rangle &= (1 - G_0 V_1)^{-1}|\phi_k\rangle = \left(1 - \lim_{\epsilon\to 0}\frac{V_1}{E + \mathrm{i}\epsilon - \hat{H}_0}\right)^{-1}|\phi_k\rangle = \lim_{\epsilon\to 0}\frac{E + \mathrm{i}\epsilon - \hat{H}_0}{E + \mathrm{i}\epsilon - \hat{H}_0 - V_1}|\phi_k\rangle \\
&= \lim_{\epsilon\to 0}\frac{E + \mathrm{i}\epsilon - \hat{H}_0}{E + \mathrm{i}\epsilon - \hat{H}_1}|\phi_k\rangle = \lim_{\epsilon\to 0}\frac{E_k + V_1 + \mathrm{i}\epsilon - E_k}{E + \mathrm{i}\epsilon - \hat{H}_1}|\phi_k\rangle = \lim_{\epsilon\to 0}\frac{V_1}{E + \mathrm{i}\epsilon - \hat{H}_1}|\phi_k\rangle = G_1 V_1|\phi_k\rangle\,.
\end{aligned}
\tag{3.134}
$$

Here, $|\phi_k\rangle$ is a momentum eigenstate of $\hat{H}_0$ with $\hat{H}_0|\phi_k\rangle = E_k|\phi_k\rangle$ and $|\phi_k^{(+)}\rangle$ is an eigenstate of the total Hamiltonian $\hat{H}_1 = \hat{H}_0 + V_1$ with $\hat{H}_1|\phi_k^{(+)}\rangle = E|\phi_k^{(+)}\rangle$. Thus, $T(k)$ can be rewritten as

$$
\begin{aligned}
T(k) &= \langle\phi_k|V_1|\psi_2 + \psi_3\rangle + \langle\phi_k|V_1 G_1 V_1|\psi_2 + \psi_3\rangle = \langle\phi_k|V_1|\psi_2 + \psi_3\rangle + \langle\phi_k|V_1|\psi_1 - \phi_1\rangle \\
&= \langle\phi_k|V_1|\Psi^{(+)}\rangle - \langle\phi_k|V_1|\phi_1\rangle\,.
\end{aligned}
\tag{3.135}
$$

The second term in the last line vanishes on-shell due to strong surface oscillations that do not contribute to the cross section. The first term is the contribution to the break-up amplitude from channel 1, because we used the form (3.62). Adding up all three channels we get the total break-up amplitude

$$
T(k) = \langle\phi_k|V_1 + V_2 + V_3|\Psi^{(+)}\rangle = \langle\phi_k|V^0|\Psi^{(+)}\rangle \tag{3.136}
$$

according to Eq (3.126) with $\beta = 0$ for the break-up channel.

4 Generalization of the Glöckle approach to three interacting distinguishable spinless particles

The total wave function $\Psi^{(+)}$ for a specific channel is again decomposed into three so called Faddeev components [8]. Each component represents a sub-system, where two particles j, k interact via a two-body potential $V_{jk}(r_i)$ and the third one moves freely. Finally all three components are summed up to get the total solution.

In Section 3.2 we could show that all three Faddeev components can be represented by *one single* component ψ after applying permutation operators and using the symmetry in the total wave function of a specific channel. The system of three coupled equations was then reduced to one single equation for $\psi(r_1, R_1)$. These arguments are no longer valid in this section as the symmetry in the total wave function gets lost when the particles are *non identical*. Therefore we have to determine three *different* Faddeev components $\psi_i(r_i, R_i)$, which depend on each other. Hence, a system of three coupled (integral or differential) equations has to be solved to get the total wave function $\Psi^{(+)}$ for a certain channel. In the R-matrix formalism we will again obtain a set of equations to determine expansion coefficients for the interior wave functions and the T_i amplitudes.

The microscopic Hamiltonian for the three-body system reads ($\hbar = 1$)

$$\hat{H}_{micr} = -\frac{1}{2m_1}\vec{\nabla}_1^2 - \frac{1}{2m_2}\vec{\nabla}_2^2 - \frac{1}{2m_3}\vec{\nabla}_3^2 + V_{23} + V_{31} + V_{12} + V_4\,, \tag{4.1}$$

where the m_i stand for the mass of the particles, respectively and the $V_{ij}\,, (i \neq j)$ denote the pair interaction between particles i and j. V_4 is the three-body force, which will not be considered in the following calculations. Following Faddeev [7] we split the total scattering wave function for a certain channel $|\Psi_\alpha^{(+)}\rangle$ into three so called Faddeev components $|\psi_\alpha\rangle_i$, where $|\Psi_\alpha^{(+)}\rangle = |\psi_\alpha\rangle_1 + |\psi_\alpha\rangle_2 + |\psi_\alpha\rangle_3$. We change from Cartesian coordinates to natural Jacobi coordinates,

$$\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \longrightarrow \mathbf{r}_i, \mathbf{R}_i, \mathbf{R}_{cm} \tag{4.2}$$

and choose the coordinate space representation $\psi_i(\mathbf{r_i}, \mathbf{R_i})_\alpha = \langle \mathbf{r_i}\mathbf{R_i}|\psi_\alpha^{(+)}\rangle_i$ for the Faddeev amplitudes $|\psi_\alpha^{(+)}\rangle_i$. Here, $\mathbf{R}_{cm}$ is the vector pointing to the center of mass is neglected since its motion is trivial. The three sets of Jacobi coordinates are defined as

$$\mathbf{r}_1 = \mathbf{x}_2 - \mathbf{x}_3\,, \qquad \mathbf{R}_1 = \mathbf{x}_1 - \frac{m_2\mathbf{x}_2 + m_3\mathbf{x}_3}{m_2 + m_3}\,, \tag{4.3}$$

$$\mathbf{r}_2 = \mathbf{x}_3 - \mathbf{x}_1\,, \qquad \mathbf{R}_2 = \mathbf{x}_2 - \frac{m_3\mathbf{x}_3 + m_1\mathbf{x}_1}{m_1 + m_3}\,, \tag{4.4}$$

$$\mathbf{r}_3 = \mathbf{x}_1 - \mathbf{x}_2\,, \qquad \mathbf{R}_3 = \mathbf{x}_3 - \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}\,, \tag{4.5}$$

where $\mathbf{x}_i$ represent Cartesian coordinates.

Each component $\psi_i(\mathbf{r_i}, \mathbf{R_i})_\alpha$ represents one subsystem (Fig. 4) and is an eigenfunction of the

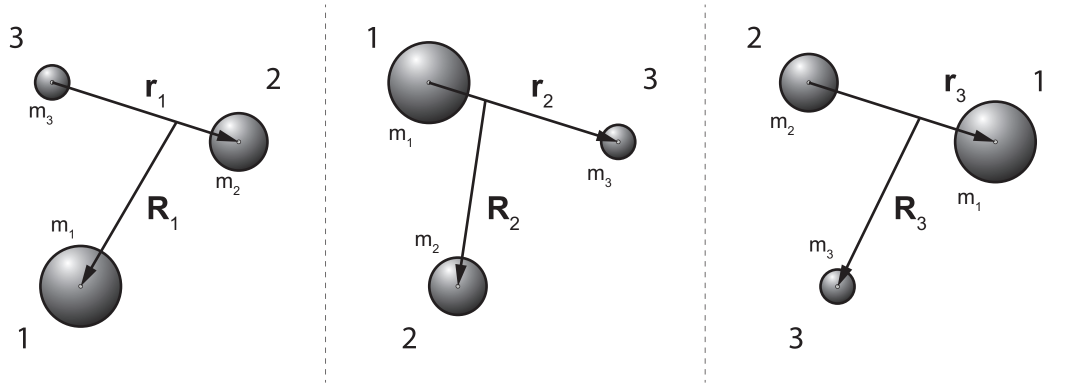

Figure 4: Three subsystems characterized by different sets of Jacobi coordinates.

corresponding Hamilton operator $\hat{H}_i$,

$$\begin{aligned}
\hat{H}_1 &= -\frac{1}{2\mu_{23}}\vec{\nabla}_{\vec{r}_1} - \frac{1}{2\mu_{1(23)}}\vec{\nabla}_{\vec{R}_1} + V_{23}(r_1)\,,\\
\hat{H}_2 &= -\frac{1}{2\mu_{31}}\vec{\nabla}_{\vec{r}_2} - \frac{1}{2\mu_{2(31)}}\vec{\nabla}_{\vec{R}_2} + V_{31}(r_2)\,,\\
\hat{H}_3 &= -\frac{1}{2\mu_{12}}\vec{\nabla}_{\vec{r}_3} - \frac{1}{2\mu_{3(12)}}\vec{\nabla}_{\vec{R}_3} + V_{12}(r_3)\,,
\end{aligned} \tag{4.6}$$

with the reduced masses

$$\begin{aligned}
\mu_{23} &= \frac{m_2 m_3}{m_2+m_3}, \quad \mu_{1(23)} = \frac{m_1(m_2+m_3)}{m_1+m_2+m_3}\,,\\
\mu_{31} &= \frac{m_3 m_1}{m_3+m_1}, \quad \mu_{2(31)} = \frac{m_2(m_3+m_1)}{m_1+m_2+m_3}\,,\\
\mu_{12} &= \frac{m_1 m_2}{m_1+m_2}, \quad \mu_{(3(12)} = \frac{m_3(m_1+m_2)}{m_1+m_2+m_3}\,.
\end{aligned} \tag{4.7}$$

Again, we have five exit channels, three two-body fragmentation channels α, β, γ (Fig. 5), the break-up channel with index 0 (Fig. 6) and a channel B where all three particles form one bound state:

1) $1\begin{pmatrix}2\\3\end{pmatrix}$ Final cannel α : Elastic channel

2) $2\begin{pmatrix}3\\1\end{pmatrix}$ Final cannel β : Rearrangement channel

3) $3\begin{pmatrix}1\\2\end{pmatrix}$ Final cannel γ : Rearrangement channel

4) $1,2,3$ Final cannel 0 : Break-up channel

5) $\begin{pmatrix}1\\2\\3\end{pmatrix}$ Final cannel B : Bound channel

The particles in the brackets in 1), 2) and 3) interact via a two-body potential $V_{jk}(r_i)$ and form a bound state. Although there exist quite a few light nuclei that can be considered as three-particle bound states, like for instance ppn $\hat{=}$ ^{3}He, pnn $\hat{=}$ ^{3}H, αnn $\hat{=}$ ^{6}He and αpn $\hat{=}$ ^{6}Li (n denotes a neutron and p a proton), we neglect channel B in this thesis.

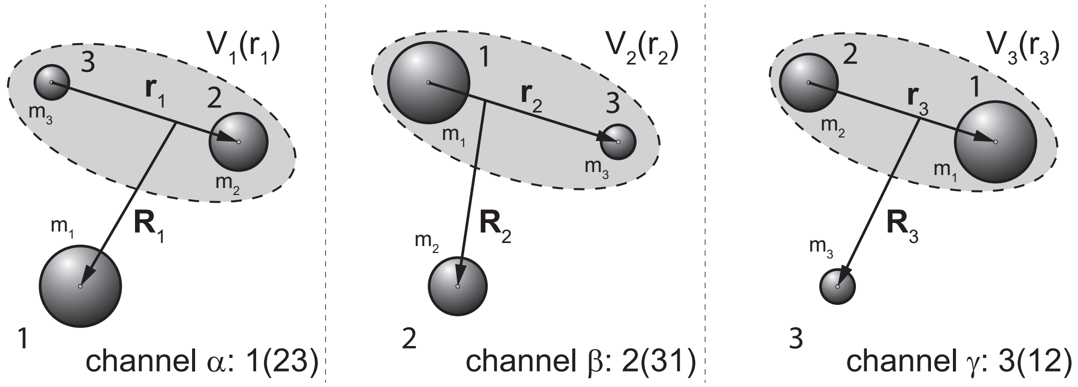

Figure 5: Two-body fragmentation channels

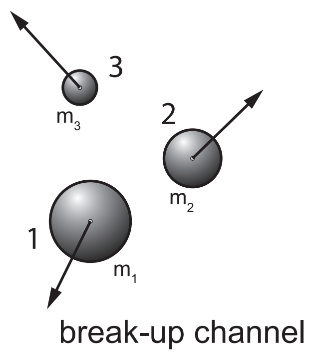

Figure 6: Break-up channel

So having, for instance, an incoming state in channel α which consists of a bound state of particles 2 and 3 and particle 1 moving freely, the scattering process can lead to four possible exit channels depicted in Figs. 5 and 6.

The Faddeev equations (3.11) in coordinate space representation for channel α read

$$\begin{aligned}
\psi_1(\mathbf{r}_1,\mathbf{R}_1)_\alpha &= \phi_1(r_1,R_1)_\alpha + \int \mathrm{d}^3r_1' \int \mathrm{d}^3R_1' \langle \mathbf{r}_1\mathbf{R}_1|G_1|\mathbf{r}_1'\mathbf{R}_1'\rangle V_{23}(r_1')[\psi_2(\mathbf{r}_2',\mathbf{R}_2')_\alpha + \psi_3(\mathbf{r}_3',\mathbf{R}_3')_\alpha]\\
\psi_2(\mathbf{r}_2,\mathbf{R}_2)_\alpha &= \int \mathrm{d}^3r_2' \int \mathrm{d}^3R_2' \langle \mathbf{r}_2\mathbf{R}_2|G_2|\mathbf{r}_2'\mathbf{R}_2'\rangle V_{31}(r_2')[\psi_1(\mathbf{r}_1',\mathbf{R}_1')_\alpha + \psi_3(\mathbf{r}_3',\mathbf{R}_3')_\alpha]\\
\psi_3(\mathbf{r}_3,\mathbf{R}_3)_\alpha &= \int \mathrm{d}^3r_3' \int \mathrm{d}^3R_3' \langle \mathbf{r}_3\mathbf{R}_3|G_3|\mathbf{r}_3'\mathbf{R}_3'\rangle V_{12}(r_3')[\psi_1(\mathbf{r}_1',\mathbf{R}_1')_\alpha + \psi_2(\mathbf{r}_2',\mathbf{R}_2')_\alpha]\,,
\end{aligned} \tag{4.8}$$

for channel β

$$\begin{aligned}
\psi_1(\mathbf{r}_1,\mathbf{R}_1)_\beta &= \int \mathrm{d}^3r_1' \int \mathrm{d}^3R_1' \langle \mathbf{r}_1\mathbf{R}_1|G_1|\mathbf{r}_1'\mathbf{R}_1'\rangle V_{23}(r_1')[\psi_2(\mathbf{r}_2',\mathbf{R}_2')_\beta + \psi_3(\mathbf{r}_3',\mathbf{R}_3')_\beta]\\
\psi_2(\mathbf{r}_2,\mathbf{R}_2)_\beta &= \phi_2(r_2,R_2)_\beta + \int \mathrm{d}^3r_2' \int \mathrm{d}^3R_2' \langle \mathbf{r}_2\mathbf{R}_2|G_2|\mathbf{r}_2'\mathbf{R}_2'\rangle V_{31}(r_2')[\psi_1(\mathbf{r}_1',\mathbf{R}_1')_\beta + \psi_3(\mathbf{r}_3',\mathbf{R}_3')_\beta]\\
\psi_3(\mathbf{r}_3,\mathbf{R}_3)_\beta &= \int \mathrm{d}^3r_3' \int \mathrm{d}^3R_3' \langle \mathbf{r}_3\mathbf{R}_3|G_3|\mathbf{r}_3'\mathbf{R}_3'\rangle V_{12}(r_3')[\psi_1(\mathbf{r}_1',\mathbf{R}_1')_\beta + \psi_2(\mathbf{r}_2',\mathbf{R}_2')_\beta]\,,
\end{aligned} \tag{4.9}$$

and for channel γ

$$\begin{aligned}
\psi_1(\mathbf{r}_1,\mathbf{R}_1)_\gamma &= \int \mathrm{d}^3r_1' \int \mathrm{d}^3R_1' \langle \mathbf{r}_1\mathbf{R}_1|G_1|\mathbf{r}_1'\mathbf{R}_1'\rangle V_{23}(r_1')[\psi_2(\mathbf{r}_2',\mathbf{R}_2')_\gamma + \psi_3(\mathbf{r}_3',\mathbf{R}_3')_\gamma]\\
\psi_2(\mathbf{r}_2,\mathbf{R}_2)_\gamma &= \int \mathrm{d}^3r_2' \int \mathrm{d}^3R_2' \langle \mathbf{r}_2\mathbf{R}_2|G_2|\mathbf{r}_2'\mathbf{R}_2'\rangle V_{31}(r_2')[\psi_1(\mathbf{r}_1',\mathbf{R}_1')_\gamma + \psi_3(\mathbf{r}_3',\mathbf{R}_3')_\gamma]\\
\psi_3(\mathbf{r}_3,\mathbf{R}_3)_\gamma &= \phi_3(r_3,R_3)_\gamma + \int \mathrm{d}^3r_3' \int \mathrm{d}^3R_3' \langle \mathbf{r}_3\mathbf{R}_3|G_3|\mathbf{r}_3'\mathbf{R}_3'\rangle V_{12}(r_3')[\psi_1(\mathbf{r}_1',\mathbf{R}_1')_\gamma + \psi_2(\mathbf{r}_2',\mathbf{R}_2')_\gamma]\,.
\end{aligned} \tag{4.10}$$

The wave function in the break-up channel again follows from coherently summing up the leading contributions of all three Faddeev components in the limit $r_i \to \infty$ and $R_i \to \infty$, which are extracted by the method of steepest descent. Again, we restrict ourselves to a total angular momentum state with $L = 0$, the s-wave part of the potential $V_{jk}(r_i)$, and define $\psi_i(r_i, R_i) = \dfrac{u_i(r_i, R_i)}{r_i R_i}$ and $x_i = \hat{\mathbf{r}}_i \cdot \hat{\mathbf{R}}_i$. Furthermore we introduce the abbreviations $V_{23}(r_1) \equiv V_1(r_1)$, $V_{31}(r_2) \equiv V_2(r_2)$ and $V_{12}(r_3) \equiv V_3(r_3)$, or generally $V_{jk}(r_i) \equiv V_i(r_i)$. This notation where the three-particles are represented by the set i, j, k will be used throughout Section 3. It enables us to establish generic results valid for all three Faddeev components and thus provides a compact way to set up a R-matrix theory for three distinguishable particles.

In channel α (the index "α" will be omitted in the following) we obtain for the Faddeev components

$$
\begin{aligned}
u_i(r_i,R_i) =& \delta_{i1} u_b(r_i)\sin(QR_i) + \int_0^\infty \mathrm{d}r_i' \int_0^\infty \mathrm{d}R_i' \, \langle r_i R_i | G_i | r_i' R_i' \rangle V_i(r_i') \\
& \times \int_{-1}^{1} \mathrm{d}x' r_i' R_i' \frac{1}{2} \left[\frac{u_j(r_j', R_j')}{r_j' R_j'} + \frac{u_k(r_k', R_k')}{r_k' R_k'} \right] \\
=& u_b(r_i)\sin(QR_i) + \int_0^\infty \mathrm{d}r_i' \int_0^\infty \mathrm{d}R_i' \, \langle r_i R_i | G_i | r_i' R_i' \rangle V_i(r_i') Q_i(r_i', R_i')
\end{aligned}
\tag{4.11}
$$

with the source term

$$
Q_i(r_i,R_i) = \int_{-1}^{1} \mathrm{d}x_i \, \frac{r_i R_i}{2} \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{u_j(r_j,R_j)}{r_j R_j} \,. \tag{4.12}
$$

For instance, the first Faddeev component is given by

$$
\begin{aligned}
u_1(r_1,R_1) =& u_1^b(r_1)\sin(QR_1) + \int_0^\infty \mathrm{d}r_1' \int_0^\infty \mathrm{d}R_1' \, \langle r_1 R_1 | G_1 | r_1' R_1' \rangle V(r_1') \\
& \times \int_{-1}^{1} \mathrm{d}x' r_1' R_1' \frac{1}{2} \left[\frac{u_2(r_2', R_2')}{r_2' R_2'} + \frac{u_3(r_3', R_3')}{r_3' R_3'} \right] \\
=& u_1^b(r_1)\sin(QR_1) + \int_0^\infty \mathrm{d}r_1' \int_0^\infty \mathrm{d}R_1' \, \langle r_1 R_1 | G_1 | r_1' R_1' \rangle V_1(r_1') Q_1(r_1', R_1') \,.
\end{aligned}
\tag{4.13}
$$

Applying $(E-\hat{H}_i)$ on both sides of Eq. (4.11) and using the identity

$$
(E-\hat{H}_i)\langle r_i R_i | G_i | r_i' R_i' \rangle = (E-\hat{H}_i)\langle r_i R_i | \frac{1}{E-\hat{H}_i} | r_i' R_i' \rangle = \delta(\mathbf{r}_i - \mathbf{r}_i')\delta(\mathbf{R}_i - \mathbf{R}_i')
$$

yields

$$
\begin{aligned}
& \left[-\frac{1}{2\mu_{jk}} \frac{\mathrm{d}^2}{\mathrm{d}r_i^2} - \frac{1}{2\mu_{i(jk)}} \frac{\mathrm{d}^2}{\mathrm{d}R_i^2} + V_i(r_i) - E \right] u_i(r_i,R_i) \\
&= -\int_0^\infty \mathrm{d}r_i' \int_0^\infty \mathrm{d}R_i' \, \delta(\mathbf{r}_i - \mathbf{r}_i')\delta(\mathbf{R}_i - \mathbf{R}_i') V_i(r_i') \int_{-1}^{1} \mathrm{d}\, x_i' \frac{r_i' R_i'}{2} \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{u_j(r_j', R_j')}{r_j' R_j'} \\
&= -\frac{1}{2} V_i(r_i) \int_{-1}^{1} \mathrm{d}x_i \, r_i R_i \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{u_j(r_j,R_j)}{r_j R_j} \,,
\end{aligned}
\tag{4.14}
$$

with boundary conditions for outgoing scattered waves.

4.1 Asymptotic behavior

In the following we introduce the polar coordinates

$$
\begin{aligned}
r_i &= \sqrt{\frac{1}{2\mu_{jk}}}\rho\cos\varphi_i\,,\\
R_i &= \sqrt{\frac{1}{2\mu_{i(jk)}}}\rho\sin\varphi_i\,.
\end{aligned} \tag{4.15}
$$

The asymptotic form of $u_i(\rho,\varphi_i)$ results to be the same as for identical particles, Eq. (3.47),

$$
u_i(\rho,\varphi_i) \underset{\substack{\rho\to\infty\\ 0<\varphi<\pi/2}}{\backsimeq} \frac{\mathrm{e}^{i\sqrt{E_i}\rho}}{\rho^{1/2}}\mathrm{A}(\varphi_i)\,. \tag{4.16}
$$

This can be verified by applying the transformation (4.15) to Eq. (4.14). In the asymptotic range ($V_i(r_i)\sim 0$) one can show that the form (4.16) fulfills the equation, which is demonstrated in Appendix A.

The energies E_i appearing in the different Faddeev components clearly have the same magnitude E, since we describe the same system, but using different sets of Jacobi coordinates in each component. The composition of each energy value E_i, however, is different and thus, we get three energy-momentum relations, each corresponding to one Faddeev component,

$$
E = E_1 = -\frac{\kappa_1^2}{2\mu_{23}} + \frac{Q_1^2}{2\mu_{1(23)}} = E_b^{(1)} + \frac{Q_1^2}{2\mu_{1(23)}} = \frac{k_1^2}{2\mu_{23}} + \frac{Q_{k_1}^2}{2\mu_{1(23)}} = \frac{q_{K_1}^2}{2\mu_{23}} + \frac{K_1^2}{2\mu_{1(23)}} \tag{4.17}
$$

$$
E = E_2 = -\frac{\kappa_2^2}{2\mu_{31}} + \frac{Q_2^2}{2\mu_{2(31)}} = E_b^{(2)} + \frac{Q_2^2}{2\mu_{2(31)}} = \frac{k_2^2}{2\mu_{31}} + \frac{Q_{k_2}^2}{2\mu_{2(31)}} = \frac{q_{K_2}^2}{2\mu_{31}} + \frac{K_2^2}{2\mu_{2(31)}} \tag{4.18}
$$

$$
E = E_3 = -\frac{\kappa_3^2}{2\mu_{12}} + \frac{Q_3^2}{2\mu_{3(12)}} = E_b^{(3)} + \frac{Q_3^2}{2\mu_{3(12)}} = \frac{k_3^2}{2\mu_{12}} + \frac{Q_{k_3}^2}{2\mu_{3(12)}} = \frac{q_{K_3}^2}{2\mu_{12}} + \frac{K_3^2}{2\mu_{3(12)}}\,. \tag{4.19}
$$

These relations can be generalized to

$$
E = E_i = -\frac{\kappa_i^2}{2\mu_{jk}} + \frac{Q_i^2}{2\mu_{i(jk)}} = E_b^{(i)} + \frac{Q_i^2}{2\mu_{i(jk)}} = \frac{k_i^2}{2\mu_{jk}} + \frac{Q_{k_i}^2}{2\mu_{i(jk)}} = \frac{q_{K_i}^2}{2\mu_{jk}} + \frac{K_i^2}{2\mu_{i(jk)}}\,. \tag{4.20}
$$

In the following, unless otherwise declared, all wavenumbers in Section 4, are related to component i and we set $Q_i\equiv Q, k_i\equiv k, Q_{k_i}\equiv Q_k, q_{k_i}\equiv q_k, K_i\equiv K$, in order to avoid confusions due to indices. In order to establish the asymptotic form of the source term $Q_i(r_i,R_i)$ (4.12) in the limit $R_i\to\infty$ and r_i fixed, we need relations that express two sets of Jacobi coordinates $\mathbf{r}_j,\mathbf{R}_j$ ($j\neq i$) as functions of the remaining one $\mathbf{r}_i,\mathbf{R}_i$. The three sets of Jacobi coordinates have been defined in Eqs. (4.3)-(4.5). For $i=1,2$ one finds ($i\neq j\neq k$ and $i\neq k$)

$$
\mathbf{r}_j = -\frac{m_j}{m_j+m_k}\mathbf{r}_i - (-1)^j\mathbf{R}_i\,, \qquad \mathbf{R}_j = (-1)^j\frac{m_im_k+m_jm_k+m_km_k}{(m_i+m_k)(m_j+m_k)}\mathbf{r}_i - \frac{m_i}{m_i+m_k}\mathbf{R}_i, \tag{4.21}
$$

and for $i = 3$ ($i \neq j \neq k$ and $i \neq k$)

$$\mathbf{r}_j = -\frac{m_j}{m_j + m_k}\mathbf{r}_i + (-1)^j \mathbf{R}_i\,, \qquad \mathbf{R}_j = -(-1)^j \frac{m_i m_k + m_j m_k + m_k m_k}{(m_i + m_k)(m_j + m_k)}\mathbf{r}_i - \frac{m_i}{m_i + m_k}\mathbf{R}_i\,. \quad (4.22)$$

For instance, if we set $i = 1$, we obtain

$$\begin{aligned} \mathbf{r}_2 &= -\frac{m_2}{m_2 + m_3}\mathbf{r}_1 - \mathbf{R}_1\,, \qquad \mathbf{R}_2 = \frac{m_1 m_3 + m_2 m_3 + m_3 m_3}{(m_1 + m_3)(m_2 + m_3)}\mathbf{r}_1 - \frac{m_1}{m_1 + m_3}\mathbf{R}_1, \\ \mathbf{r}_3 &= -\frac{m_3}{m_2 + m_3}\mathbf{r}_1 + \mathbf{R}_1\,, \qquad \mathbf{R}_3 = -\frac{m_1 m_2 + m_2 m_2 + m_3 m_2}{(m_1 + m_2)(m_2 + m_3)}\mathbf{r}_1 - \frac{m_1}{m_1 + m_2}\mathbf{R}_1\,, \end{aligned} \quad (4.23)$$

which is the generalized form of Eq. (3.24) for three distinguishable particles. The magnitudes for ($x_i = \hat{\mathbf{r}}_i \cdot \hat{\mathbf{R}}_i$) are

$$\begin{aligned} r_j(x_i) &= \sqrt{\left(\frac{m_j}{m_j + m_k} r_i\right)^2 + R_i^2 + 2\frac{(-1)^j m_j}{m_j + m_k} r_i R_i x_i} = R_i \sqrt{1 + \left(\frac{m_j}{m_j + m_k}\right)^2 \frac{r_i^2}{R_i^2} + 2\frac{(-1)^j m_j}{m_j + m_k}\frac{r_i}{R_i} x_i} \\ &\approx R_i \left(1 + (-1)^j \frac{m_j}{m_j + m_k}\frac{r_i}{R_i} x_i + ...\right) = R_i + (-1)^j \frac{m_j}{m_j + m_k} r_i x_i + ... \\ R_j(x_i) &= \sqrt{\left(\frac{m_i m_k + m_j m_k + m_k m_k}{(m_i + m_k)(m_j + m_k)} r_i\right)^2 + \left(\frac{m_i}{m_i + m_k} R_i\right)^2 - \frac{2(-1)^j m_i (m_i m_k + m_j m_k + m_k m_k)}{(m_i + m_k)(m_i + m_k)(m_j + m_k)} R_i r_i x_i} \\ &= \frac{m_i R_i}{m_i + m_k} \\ &\times \sqrt{1 + \left(\frac{(m_i + m_k)(m_i m_k + m_j m_k + m_k m_k)}{m_i (m_i + m_k)(m_j + m_k)}\frac{r_i}{R_i}\right)^2 - \frac{2(-1)^j (m_i + m_k)(m_i m_k + m_j m_k + m_k m_k)}{m_i (m_i + m_k)(m_j + m_k)}\frac{r_i x_i}{R_i}} \\ &\approx \frac{m_i}{m_i + m_k} R_i \left(1 - (-1)^j \frac{(m_i + m_k)(m_i m_k + m_j m_k + m_k m_k)}{m_i (m_i + m_k)(m_j + m_k)}\frac{r_i}{R_i} x_i + ...\right) \\ &= \frac{m_i}{m_i + m_k} R_i - (-1)^j \frac{m_i m_k + m_j m_k + m_k m_k}{(m_i + m_k)(m_j + m_k)}\frac{r_i}{R_i} x_i + ...\,, \end{aligned} \quad (4.24)$$

where $i=1,2$ ($i \neq j \neq k$ and $i \neq k$) and

$$
\begin{aligned}
r_j(x_i) &= \sqrt{\left(\frac{m_j}{m_j+m_k}r_i\right)^2 + R_i^2 - 2\frac{(-1)^j m_j}{m_j+m_k}r_i R_i x_i} = R_i\sqrt{1+\left(\frac{m_j}{m_j+m_k}\right)^2\frac{r_i^2}{R_i^2} - 2\frac{(-1)^j m_j}{m_j+m_k}\frac{r_i}{R_i}x_i} \\
&\approx R_i\left(1-(-1)^j\frac{m_j}{m_j+m_k}\frac{r_i}{R_i}x_i+...\right) = R_i - (-1)^j\frac{m_j}{m_j+m_k}r_i x_i + ... \\
R_j(x_i) &= \sqrt{\left(\frac{m_i m_k + m_j m_k + m_k m_k}{(m_i+m_k)(m_j+m_k)}r_i\right)^2 + \left(\frac{m_i}{m_i+m_k}R_i\right)^2 + \frac{2(-1)^j m_i(m_i m_k + m_j m_k + m_k m_k)}{(m_i+m_k)(m_i+m_k)(m_j+m_k)}R_i r_i x_i} \\
&= \frac{m_i R_i}{m_i+m_k} \\
&\times\sqrt{1+\left(\frac{(m_i+m_k)(m_i m_k + m_j m_k + m_k m_k)}{m_i(m_i+m_k)(m_j+m_k)}\frac{r_i}{R_i}\right)^2 + \frac{2(-1)^j(m_i+m_k)(m_i m_k + m_j m_k + m_k m_k)}{m_i(m_i+m_k)(m_j+m_k)}\frac{r_i x_i}{R_i}} \\
&\approx \frac{m_i}{m_i+m_k}R_i\left(1+(-1)^j\frac{(m_i+m_k)(m_i m_k + m_j m_k + m_k m_k)}{m_i(m_i+m_k)(m_j+m_k)}\frac{r_i}{R_i}x_i+...\right) \\
&= \frac{m_i}{m_i+m_k}R_i + (-1)^j\frac{m_i m_k + m_j m_k + m_k m_k}{(m_i+m_k)(m_j+m_k)}\frac{r_i}{R_i}x_i + ...\,,
\end{aligned}
\tag{4.25}
$$

for $i=3$ ($i \neq j \neq k$ and $i \neq k$). The expansions in Eqs. (4.24) and (4.25) are valid in the case $R_1 \to \infty$. For the asymptotic form of the source term $Q_i(r_i, R_i)$ we approximate the quantities $r_j(x_i), R_j(x_i)$ by the first term of their Taylor series. Thus, for the following we do not distinguish between the two cases $i=1,2$ and $i=3$, because in this approximation we find unique relations for the magnitudes, $r_j(x_i) \approx R_i,\ R_j(x_i) \approx \frac{m_i}{m_i+m_k}R_i$ with $i=1,2,3$. After changing to polar coordinates

$$
\begin{aligned}
r_j &= \sqrt{\frac{1}{2\mu_{ik}}}\rho\cos\varphi_j\,, \\
R_j &= \sqrt{\frac{1}{2\mu_{j(ik)}}}\rho\sin\varphi_j\,,
\end{aligned}
\tag{4.26}
$$

these first order approximations fix the angles φ_j to a constant value, depending on the reduced masses,

$$
\tan\varphi_j^* = \sqrt{\frac{\mu_{j(ik)}}{\mu_{ik}}}\frac{R_j}{r_j} \approx \frac{m_i}{m_i+m_k}\sqrt{\frac{\mu_{j(ik)}}{\mu_{ik}}} \Rightarrow \varphi_j^* = \arctan\left(\frac{m_i}{m_i+m_k}\sqrt{\frac{\mu_{j(ik)}}{\mu_{ik}}}\right)\,. \tag{4.27}
$$

In the asymptotic form of $Q_i(r_i, R_i)$ we replace the Faddeev components $u_j(r_j, R_j)$ by their asymptotic form (4.16), which is justified, since $R_i \to \infty$ implies r_j and R_j tending towards infinity. Including Eq. (4.26) and the first order approximations for r_j and R_j from above, we can calculate $Q_i(r_i, R_i)$

in the limit $R_i \to \infty$ and r_i fixed,

$$
\begin{aligned}
Q_i(r_i, R_i) &= \int_{-1}^{1} \mathrm{d}x_i \; r_i R_i \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{u_j(r_j, R_j)}{r_j(x_i) R_j(x_i)} \\
&\underset{\substack{R_i \to \infty \\ r_i \text{fixed}}}{\simeq} \int_{-1}^{1} \mathrm{d}x_i \; r_i R_i \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{\mathrm{e}^{\mathrm{i}\sqrt{E}\sqrt{2\mu_{j(ik)}} R_2(x)/\sin\varphi_j}}{r_2(x) R_2(x) (2\mu_{j(ik)})^{1/4} \sqrt{\frac{R_2(x)}{\sin\varphi_j}}} \mathrm{A}(\varphi_j) \\
&= \int_{-1}^{1} \mathrm{d}x_i \; r_i R_i \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i \frac{m_i}{m_i+m_k} R_i (2\mu_{j(ik)})^{1/4} \sqrt{R_i \frac{m_i}{m_i+m_k} / \sin\varphi_2^*}} \mathrm{A}(\varphi_j^*) \\
&= \frac{r_i}{R_i^{3/2} m_i} \sum_{\substack{j=1 \\ j\neq i}}^{3} (2\mu_{j(ik)})^{-1/4} (m_i + m_k) \sqrt{\frac{m_i + m_k}{m_i} \sin\varphi_j^*} \; \mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*} \mathrm{A}(\varphi_j^*) \,.
\end{aligned}
\tag{4.28}
$$

We know two different representations of the Green's function, suitable to establish two different asymptotic forms of u, $R_1 \to \infty$, r_1 fixed and $r_1 \to \infty$, R_1 fixed, respectively. The matrix element in coordinate space representation reads

$$
\begin{aligned}
\langle r_i R_i | G_i | r_i' R_i' \rangle =& u_i^b(r_i) \left(-2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}QR_{i>}} \frac{\sin(QR_{i<})}{Q} \right) u_i^b(r_i') \\
&+ \frac{2}{\pi} \int_0^\infty \mathrm{d}k \; u_k^{(-)}(r_i) \left(-2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}Q_k R_{i>}} \frac{\sin(Q_k R_{i<})}{Q_k} \right) u_k^{(-)*}(r_i') \qquad (4.29\mathrm{a}) \\
=& \frac{2}{\pi} \int_0^\infty \mathrm{d}K \; \sin(KR_i) \left(-\frac{2\mu_{jk}}{q_K} u_{q_K}^{(+)}(r_{i<}) w_{q_K}(r_{i>}) \right) \sin(KR_i') \,, \qquad (4.29\mathrm{b})
\end{aligned}
$$

where $R_{i>} = \max(R_i, R_i')$, $R_{i<} = \min(R_i, R_i')$ and $r_{i>} = \max(r_i, r_i')$, $r_{i<} = \min(r_i, r_i')$ and i, m, n denote the different particles ($i \neq j \neq k$ and $i \neq k$), respectively. The functions $u_{qK}^{(\pm)}(r)$ and $w_{q_K}(r)$ form a complete set of bound- and scattering states and are normalized as $u_q^{(\pm)}(r) \simeq \mathrm{e}^{\pm\mathrm{i}\delta(q)} \sin(qr + \delta(q))$ and $w_q(r) \simeq \mathrm{e}^{\mathrm{i}qr}$ for $r \to \infty$. However, these expressions are only valid if Coulomb interaction is neglected. Inserting the form (4.29a) of the Green's function into Eq. (4.11) we obtain the asymptotic form of $u_i(r_i, R_i)$ in the limit $R_i \to \infty$, r_i fixed,

$$
\begin{aligned}
u_i(r_i, R_i) =& u_i^b(r_i)\sin(QR_i) - 2\mu_{i(jk)} u_i^b(r_i) \mathrm{e}^{\mathrm{i}QR_i} \int_0^{R_i} \mathrm{d}R_i' \, \frac{\sin(QR_i')}{Q} \int_0^{\infty} \mathrm{d}r_i' \, u_i^b(r_i') V_i(r_i') Q_i(r_i', R_i') \\
& - 2\mu_{i(jk)} u_i^b(r_i) \frac{\sin(QR_i)}{Q} \int_{R_i}^{\infty} \mathrm{d}R_i' \, \mathrm{e}^{\mathrm{i}QR_i'} \int_0^{\infty} \mathrm{d}r_i' \, u_i^b(r_i') V(r_i') Q(r_i', R_i') \\
& - \frac{4\mu_{i(jk)}}{\pi} \int_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \, u_k^{(-)}(r_i) \mathrm{e}^{\mathrm{i}Q_k R_i} \int_0^{R_i} \mathrm{d}R_i' \, \frac{\sin(Q_k R_i')}{Q_k} \int_0^{\infty} \mathrm{d}r_i' \, u_k^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \\
& - \frac{4\mu_{i(jk)}}{\pi} \int_{\sqrt{2\mu_{jk}E}}^{\infty} \mathrm{d}k \, u_k^{(-)}(r_i) \mathrm{e}^{\mathrm{i}Q_k R_i} \int_0^{R_i} \mathrm{d}R_i' \, \frac{\sin(Q_k R_i')}{Q_k} \int_0^{\infty} \mathrm{d}r_i' \, u_k^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \\
& - \frac{4\mu_{i(jk)}}{\pi} \int_0^{\infty} \mathrm{d}k \, u_k^{(-)}(r_i) \frac{\sin(Q_k R_i')}{Q_k} \int_{R_i}^{\infty} \mathrm{d}R_i' \, \mathrm{e}^{\mathrm{i}Q_k R_i} \int_0^{\infty} \mathrm{d}r_i' \, u_k^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \, .
\end{aligned}
\tag{4.30}
$$

In compliance with Subsection 3.2.1, the last term in Eq. (4.30) can be neglected for $R_i \to \infty$. We find three flux conserving terms in Eq. (4.30), the first, second and fourth term. These terms describe the incoming state, elastic and rearrangement processes (T_i^b) and break-up scattering ($T_i(k)$). The T-amplitudes are defined in Eqs. (4.33) and (4.34) below. The third term without the binding wavefunction $u_i^b(r_i)$ and the

$$
\begin{aligned}
H_i^{(1)}(R_i) =& 2\mu_{i(jk)} \int_{R_i}^{\infty} \mathrm{d}R_i' \, \frac{\sin[Q(R_i - R_i')]}{Q} \int_0^{\infty} \mathrm{d}r_i' \, r_i' u_i^b(r_i') V_i(r_i') Q_i(r_i', R_i') \\
\backsimeq & \sum_{\substack{j=1 \\ j\neq i}}^{3} (2\mu_{j(ik)})^{-1/4} \left(\frac{m_i + m_k}{m_i} \sin\varphi_j^* \right)^{5/2} \mathrm{A}(\varphi_j^*) \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\,\frac{m_i}{m_i+m_k} R_i / \sin\varphi_j^*}}{R_i^{3/2}} \\
& \times \frac{2\mu_{i(jk)}}{\mu_{j(ik)} \left(E - \frac{2Q^2}{\mu_{j(ik)}} \sin^2\varphi_j^* \right)} \int_0^{r_{0i}} \mathrm{d}r_i' \, r_i' u_i^b(r_i') V_i(r_i') \, ,
\end{aligned}
\tag{4.31}
$$

and the fifth term

$$
\begin{aligned}
H_i^{(2)}(r_i,R_i) =& -\frac{4\mu_{i(jk)}}{\pi}\int\limits_{\sqrt{2\mu_{jk}E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_i)\mathrm{e}^{\mathrm{i}Q_kR_i}\int\limits_0^{R_i}\mathrm{d}R_i'\,\frac{\sin(Q_kR_i')}{Q_k}\int\limits_0^{\infty}\mathrm{d}r_i'\; u_k^{(-)*}(r_i')V_i(r_i')Q_i(r_i',R_i') \\
\backsimeq& -\frac{4}{\pi}\sum_{\substack{j=1\\ j\neq i}}^{3}\left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
&\times\int\limits_{\sqrt{2\mu_{jk}E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_i)\frac{1}{\frac{1}{\mu_{jk}}k^2-2E+2\frac{\mu_{j(ik)}}{\mu_{i(jk)}}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\int\limits_0^{r_{0i}}\mathrm{d}r_i'\; u_k^{(-)*}(r_i')V(r_i') \\
&+O\left(\frac{1}{R_i^2}\right),
\end{aligned}
\tag{4.32}
$$

are treated separately. We make use of the asymptotic form (4.28) of the source term $Q_i(r_i,R_i)$ in both, $H_i^{(1)}(R_i)$ and $H_i^{(2)}(r_i,R_i)$. This is justified, since $R_i\to\infty$ implies large values for R_i' in the respective integration intervals, while r_1' is bounded by the maximum range r_{0i} of the potential V_i. Detailed calculations are carried out in Appendix F.

Introducing the T-amplitudes

$$
T_i^b = \int\limits_0^{\infty}\mathrm{d}R\int\limits_0^{\infty}\mathrm{d}r\;\frac{\sin(QR)}{Q}u_i^b(r)V_i(r)Q_i(r,R) \tag{4.33}
$$

and

$$
T_i(k) = \int\limits_0^{\infty}\mathrm{d}R\int\limits_0^{\infty}\mathrm{d}r\;\frac{\sin(Q_kR)}{Q_k}u_k^{(-)*}(r)V_i(r)Q_i(r,R)\,. \tag{4.34}
$$

and the numbers

$$
C_i^b = \left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\sin\varphi_j^*\right)^{5/2}\mathrm{A}(\varphi_j^*)\frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E-\frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)}\int\limits_0^{\infty}\mathrm{d}r\; u_i^b(r)V_i(r)\,, \tag{4.35}
$$

and

$$
\begin{aligned}
C_i(k) =& \left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\frac{1}{\frac{1}{\mu_{jk}}k^2-2E+2\frac{\mu_{j(ik)}}{\mu_{i(jk)}}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2} \\
&\times\int\limits_0^{\infty}\mathrm{d}r\; u_k^{(-)*}(r)V_i(r)\,.
\end{aligned}
\tag{4.36}
$$

enables us to write the Faddeev component $u_i(r_i,R_i)$ in the limit $R_1\to\infty$ and r_1 fixed in a compact form

$$u_i(r_i,R_i) \backsimeq u_i^b(r_i)\sin(QR_i) - 2\mu_{i(jk)}u_i^b(r_i)\mathrm{e}^{\mathrm{i}QR_i}T_i^b - \frac{4}{\pi}\mu_{i(jk)}\int\limits_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k\; u_k^{(-)}(r_i)\mathrm{e}^{\mathrm{i}Q_kR_i}T_i(k)$$
$$- \sum_{\substack{j=1\\ j\neq i}}^{3} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} \left(u_i^b(r_i)C_i^b + \frac{2}{\pi}\int\limits_{\sqrt{2\mu_{jk}E}}^{\infty} \mathrm{d}k\; u_k^{(-)}(r_i)C_i(k)\right) + O\left(\frac{1}{R_i^2}\right). \tag{4.37}$$

T_i^b and $T_i(k)$ contain the source term $Q_i(r_i,R_i)$ (4.12), which in turn is made up of the sum of Faddeev amplitudes, $\sum_{\substack{j=1\\ j\neq i}}^{3} u_j(r_j,R_j)$. Thus, the three u_i depend on each other which is a crucial difference to the case of three interacting *identical* particles. The last two terms of Eq. (4.37) are of higher order as they are based on the sum of the asymptotic forms of u_j which (in their functional form) are essentially the same for all three Faddeev components. Therefore these terms do not lead to a coupling between the u_i.
In order to obtain a form of $u_i(r_i,R_i)$ convenient to study the limit $r_i\to\infty$ and R_i fixed, we insert the form (4.29b) of the Green's function into Eq. (4.11) which yields

$$\begin{aligned}
u_i(r_i,R_i) = &-\frac{4\mu_{jk}}{\pi}\int\limits_0^{\sqrt{2\mu_{i(jk)}E}} \mathrm{d}K\;\sin(KR_i)w_{q_K}(r_i)\int\limits_0^{r_i}\mathrm{d}r_i'\;\frac{u_{q_K}^{(+)}(r_i')}{q_K}\int\limits_0^{\infty}\mathrm{d}R_i'\;\sin(KR_i')V_i(r_i')Q_i(r_i',R_i')\\
&-\frac{4\mu_{jk}}{\pi}\int\limits_{\sqrt{2\mu_{i(jk)}E}}^{\infty} \mathrm{d}K\;\sin(KR_i)w_{q_K}(r_i)\int\limits_0^{r_i}\mathrm{d}r_i'\;\frac{u_{q_K}^{(+)}(r_i')}{q_K}\int\limits_0^{\infty}\mathrm{d}R_i'\;\sin(KR_i')V_i(r_i')Q_i(r_i',R_i')\\
&-\frac{4\mu_{jk}}{\pi}\int\limits_0^{\sqrt{2\mu_{i(jk)}E}} \mathrm{d}K\;\sin(KR_i)u_{q_K}^{(+)}(r_i)\int\limits_{r_i}^{\infty}\mathrm{d}r_i'\;\frac{w_{q_K}(r_i')}{q_K}\int\limits_0^{\infty}\mathrm{d}R_i'\;\sin(KR_i')V_i(r_i')Q_i(r_i',R_i')\\
&-\frac{4\mu_{jk}}{\pi}\int\limits_{\sqrt{2\mu_{i(jk)}E}}^{\infty} \mathrm{d}K\;\sin(KR_i)u_{q_K}^{(+)}(r_i)\int\limits_{r_i}^{\infty}\mathrm{d}r_i'\;\frac{w_{q_K}(r_i')}{q_K}\int\limits_0^{\infty}\mathrm{d}R_i'\;\sin(KR_i')V_i(r_i')Q_i(r_i',R_i')\,.
\end{aligned} \tag{4.38}$$

The last two terms in Eq. (4.38), where $r_i' > r_i$, vanish in the limit $r_i\to\infty$ (see Subsection 3.2.1). The K-integration interval in the second term determines the wavenumber q_K to be complex, which can be seen from the relation $E = \dfrac{q_K^2}{2\mu_{jk}} + \dfrac{K^2}{2\mu_{i(jk)}}$. Its leading behavior results from $q_K \approx 0$ and after [6], can be estimated to be of the order of $O\left(\frac{1}{r_i^2}\right)$. With the asymptotic form $w_q(r) \backsimeq \mathrm{e}^{\mathrm{i}qr}$ of the scattering state function $w_q(r)$ we can finally write Eq. (4.38) in the form

$$u_i(r_i, R_i) \backsimeq -\frac{4\mu_{jk}}{\pi} \int_0^{\sqrt{2\mu_{i(jk)}E}} \mathrm{d}K \; \sin(KR_i)\mathrm{e}^{\mathrm{i}q_K r_i}\overline{T_i}(K) + O\left(\frac{1}{r_i^2}\right) , \tag{4.39}$$

with

$$\overline{T_i}(K) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \; \sin(KR)\frac{u_{q_K}^{(+)}}{q_K} V_i(r)Q_i(r, R) . \tag{4.40}$$

Again we can find some relation between the functions $T_i(k)$ and $\overline{T_i}(K)$. First we consider $T_i(k)$ as a function of q_K,

$$T_i(q_K) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \; \frac{u_{q_K}^{(-)*}(r)}{Q_{q_K}} \sin(Q_{q_K}R)V_i(r)Q_i(r, R) \tag{4.41}$$

and from

$$E = \frac{k^2}{2\mu_{jk}} + \frac{Q_k^2}{2\mu_{i(jk)}} = \frac{q_K^2}{2\mu_{jk}} + \frac{K^2}{2\mu_{i(jk)}} \tag{4.42}$$

we can identify $Q_{q_K} \equiv K$. This leads to

$$T_i(q_K) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \; \frac{u_{q_K}^{(-)*}(r)}{K} \sin(KR)V_i(r)Q_i(r, R) \tag{4.43}$$

and finally one finds the relation

$$\overline{T_i}(K) = \frac{K}{q_K} T_i(q_K) . \tag{4.44}$$

In an asymptotic area where $r_i \to \infty$ and R_i is fixed, $T_i(q_K)$ and $T_i(k)$ become equal, what we already argued in Subsection 3.2.1. Hence, Eq. (4.39) becomes

$$\begin{aligned}
u_i(r_i, R_i) &\backsimeq -\frac{4\mu_{jk}}{\pi} \int_0^{\sqrt{2\mu_{i(jk)}E}} \mathrm{d}K_i \; \sin(KR_i)\mathrm{e}^{\mathrm{i}q_K r_i}\overline{T_i}(K) + O\left(\frac{1}{r_i^2}\right) \\
&= -\frac{4\mu_{jk}}{\pi} \int_0^{\sqrt{2\mu_{i(jk)}E}} \mathrm{d}K \; \sin(KR_i)\mathrm{e}^{\mathrm{i}q_K r_i}\frac{K}{q_K} T(q_K) + O\left(\frac{1}{r_i^2}\right) \\
&= -\frac{4\mu_{jk}}{\pi} \int_{\sqrt{2\mu_{jk}E}}^0 \mathrm{d}q_K \; \left(-\frac{\mu_{i(jk)}}{\mu_{jk}}\right) \frac{q_K}{K} \sin(KR_i)\mathrm{e}^{\mathrm{i}q_K r_i}\frac{K}{q_K} T(q_K) + O\left(\frac{1}{r_i^2}\right) \\
&= -\frac{4\mu_{i(jk)}}{\pi} \int_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \; \sin(KR_i)\mathrm{e}^{\mathrm{i}kr_i} T_i(k) + O\left(\frac{1}{r_i^2}\right) .
\end{aligned} \tag{4.45}$$

In the second line of Eq. (4.45) we made use of Eq. (4.44). Then the integration variable K was transformed to q_K according to relation (4.42) and

$$\begin{aligned} 0 &= \frac{1}{2\mu_{jk}} 2q_K \mathrm{d}q_K + \frac{1}{2\mu_{i(jk)}} 2K\mathrm{d}K \\ \mathrm{d}K &= -\frac{\mu_{i(jk)}}{\mu_{jk}} \frac{q_K}{K} \mathrm{d}q_K \,. \end{aligned} \tag{4.46}$$

In the last line of Eq. (4.45) we used the asymptotic equality of q_K and k. Next, we want to extract the leading behavior of the Faddeev amplitudes in the break-up channel, that means $r_i \to \infty$ and $R_i \to \infty$. Again, this is achieved by the method of integration along the line of steepest descent [11], also known as the saddle point method. This is a generalization of Laplace's method for integrals in the complex plane. Before applying it to the wave functions $u_i(r_i, R_i)$, it is useful to transform both, Jacobi coordinates and momenta, into polar coordinates.

$$\begin{aligned} r_i &= \sqrt{\frac{1}{2\mu_{jk}}} \rho \cos\varphi_i \,, & q_K &= \sqrt{2\mu_{jk}E} \cos\alpha \,, \\ R_i &= \sqrt{\frac{1}{2\mu_{i(jk)}}} \rho \sin\varphi_i \,, & K &= \sqrt{2\mu_{i(jk)}E} \sin\alpha \,. \end{aligned} \tag{4.47}$$

Starting with Eq. (4.39), we get

$$\begin{aligned} u_i(r_i, R_i) &\backsimeq -\frac{4\mu_{jk}}{\pi} \int\limits_0^{\sqrt{2\mu_{i(jk)}E}} \mathrm{d}K \; \sin(KR_i) \mathrm{e}^{\mathrm{i}q_K r_i} \overline{T_i}(K) \\ &= -\frac{4\mu_{jk}}{\pi} \sqrt{2\mu_{i(jk)}E} \int\limits_0^{\pi/2} \mathrm{d}(\sin\alpha) \; \sin(\rho \sin\alpha \cdot \sin\varphi_i) \mathrm{e}^{\mathrm{i}\rho\cos\varphi_i \cdot \cos\alpha} \overline{T_i}\left(\sqrt{2\mu_{i(jk)}E}\sin\alpha\right) \end{aligned} \tag{4.48}$$

With regard to its functional form the integrand of Eq. (4.48) is the same as in I_2 in Eq. (3.75), which is treated in Appendix C. Analogously we get

$$I_i^{(2)} = -\frac{2\mu_{jk}}{\pi \mathrm{i}} \sqrt{2\mu_{i(jk)}E} \int\limits_{-\pi/2}^{\pi/2} \mathrm{d}\alpha \; \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha - \varphi_i)} \cos\alpha \; \overline{T_i}\left(\sqrt{2\mu_{i(jk)}E}\sin\alpha\right) \,. \tag{4.49}$$

In order to extract the leading behavior for $\rho \to \infty$, which implies $r_i \to \infty$ and $R_i \to \infty$, the formalism of the saddle point method can be applied. In analogy to Subsection 3.2.1 one obtains

$$
\begin{aligned}
I_i^{(2)} \backsimeq & \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} 2\mu_{jk} \sqrt{2\mu_{i(jk)}E} \frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}} \\
& \times \left[\cos\varphi_i \, \overline{T_i} \left(\sqrt{2\mu_{1(23)}E}\sin\varphi_i\right) - \frac{\mathrm{i}}{2}\frac{1}{\rho\sqrt{E}}\frac{\mathrm{d}^2}{\mathrm{d}\varphi_i^2}\cos\varphi_i \, \overline{T_i}\left(\sqrt{2\mu_{1(23)}E}\sin\varphi_i\right) + ... \right] .
\end{aligned}
\tag{4.50}
$$

The second term again vanishes in higher order for $\varphi_i \to 0$. This can be shown by transforming the wavenumbers in $I_i^{(2)}$ only and leaving the spatial coordinates unchanged,

$$
I_i^{(2)} = -\frac{4\mu_{jk}}{\pi}\sqrt{2\mu_{i(jk)}E} \int_0^{\pi/2} \mathrm{d}\alpha \, \sin\left(\sqrt{2\mu_{i(jk)}E} R_i \sin\alpha\right) \mathrm{e}^{\mathrm{i}r_1\sqrt{E}\cos\alpha} \cos\alpha \, \overline{T_i}\left(\sqrt{2\mu_{i(jk)}E}\sin\alpha\right) .
\tag{4.51}
$$

Then one integrates along the line of steepest descent starting from $\alpha = 0$ and obtains exactly the same result when expanding the first term of Eq. (4.50) for $\varphi_i \to 0$. Consequently the second derivative term in Eq. (4.50) must vanish in higher order for $\varphi_i \to 0$. A more detailed treatment is presented in Subsection 3.2.1.

Another possible way to derive the leading behavior of $u_i(r_i, R_i)$ in the break-up channel is to use the form

$$
\begin{aligned}
I_i^{(1)} &= -\frac{4\mu_{i(jk)}}{\pi} \int_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \; u_k^{(-)}(r_i) \mathrm{e}^{\mathrm{i}Q_k R_i} T_i(k) \\
&= -\frac{4\mu_{i(jk)}}{\pi} \int_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \; \mathrm{e}^{-\mathrm{i}\delta(k)} \sin(kr_i + \delta(k)) \mathrm{e}^{\mathrm{i}Q_k R_i} T_i(k) \, ,
\end{aligned}
\tag{4.52}
$$

which is part of u_i in the limit $R_i \to \infty$ and r_i fixed (Eq. (4.37)). Clearly, the binding wave functions $u_i^b(r_i)$ vanish in the break-up channel and $u_k^{(-)}(r_i)$ is replaced by its asymptotic form $u_k^{(-)}(r_i) \backsimeq \mathrm{e}^{-\mathrm{i}\delta(k)}\sin(kr_i + \delta(k))$ since both Jacobi variables tend towards infinity. Again we transform the integral according to

$$
\begin{aligned}
r_i &= \sqrt{\frac{1}{2\mu_{jk}}}\rho\sin\beta_i \, , & k &= \sqrt{2\mu_{jk}E}\sin\vartheta \, , \\
R_i &= \sqrt{\frac{1}{2\mu_{i(jk)}}}\rho\cos\beta_i \, , & Q_k &= \sqrt{2\mu_{i(jk)}E}\cos\vartheta \, ,
\end{aligned}
\tag{4.53}
$$

which results in

$$I_i^{(1)} = -\frac{4\mu_{i(jk)}}{\pi}\sqrt{2\mu_{jk}E}\int\limits_0^{\pi/2} \mathrm{d}\vartheta\ \cos\vartheta\, \mathrm{e}^{-\mathrm{i}\delta(\sqrt{2\mu_{jk}E}\sin\vartheta)}\sin(\sqrt{E}\sin\beta_i\sin\vartheta + \delta(\sqrt{2\mu_{jk}E}\sin\vartheta))$$
$$\times\, \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos\beta_i\cos\vartheta}T_i\left(\sqrt{2\mu_{jk}E}\sin\vartheta\right) . \tag{4.54}$$

This is exactly the same form as found for I_1 in Subsection 3.2.1. Hence, the integral in Eq. (4.54) can similarly be treated as in Appendix D, which results in

$$I_i^{(1)} = -\frac{2\mu_{i(jk)}}{\pi\mathrm{i}}\sqrt{2\mu_{jk}E}\int\limits_{-\pi/2}^{\pi/2} \mathrm{d}\vartheta\ \cos\vartheta\, \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta_i)}T_i\left(\sqrt{2\mu_{jk}E}\sin\vartheta\right) . \tag{4.55}$$

The asymptotic behavior of I_1 is again dominated by the contribution from the saddlepoint $\vartheta = \beta_i$ and can be calculated in the frame of the method of steepest descent. We set $\vartheta = \beta_i = \frac{\pi}{2} - \varphi_i$ and after integration along the path of steepest descent we obtain

$$I_i^{(1)} \backsimeq 2\mu_{i(jk)}\sqrt{\frac{1}{\pi\mathrm{i}}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\sqrt{2\mu_{jk}E}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}}$$
$$\times\left[\sin\varphi_i\ T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right) - \frac{\mathrm{i}}{2}\frac{1}{\rho\sqrt{E}}\frac{\mathrm{d}^2}{\mathrm{d}\varphi_i^2}\sin\varphi_i\ T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right) + ...\right] . \tag{4.56}$$

This result is - as expected - closely related to Eq. (4.50) and by applying relation (4.44) in the form $\overline{T_i}\left(\sqrt{2\mu_{i(jk)}E}\sin\varphi_i\right) = \frac{\sqrt{\mu_{i(jk)}}}{\sqrt{\mu_{jk}}}\frac{\sin\varphi_i}{\cos\varphi_i}T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right)$ to (4.50), one can show the equality of both results,

$$\begin{aligned}
I_i^{(2)} \backsimeq&\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}2\mu_{jk}\sqrt{2\mu_{i(jk)}E}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}}\left[\cos\varphi_i\ \frac{\sqrt{\mu_{i(jk)}}}{\sqrt{\mu_{jk}}}\frac{\sin\varphi_i}{\cos\varphi_i}T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right)\right.\\
&\left.-\frac{\mathrm{i}}{2}\frac{1}{\rho\sqrt{E}}\frac{\mathrm{d}^2}{\mathrm{d}\varphi_i^2}\cos\varphi_i\ \frac{\sqrt{\mu_{i(jk)}}}{\sqrt{\mu_{jk}}}\frac{\sin\varphi_i}{\cos\varphi_i}T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right) + ...\right]\\
=&2\mu_{i(jk)}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\sqrt{2\mu_{jk}E}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\left(\rho\sqrt{E}\right)^{1/2}}\left[\sin\varphi_i\ T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right)\right.\\
&\left.-\frac{\mathrm{i}}{2}\frac{1}{\rho\sqrt{E}}\frac{\mathrm{d}^2}{\mathrm{d}\varphi_i^2}\sin\varphi_i\ T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right) + ...\right] = I_1 .
\end{aligned} \tag{4.57}$$

The second derivative term vanishes for $\varphi_i \to 0$.

Hence, we found the Faddeev amplitude $u_i(r_i, R_i)$ in the break-up channel,

$$u_i(r_i, R_i) \underset{\rho\to\infty}{\backsimeq} 2\mu_{i(jk)}\sqrt{2\mu_{jk}}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}}\sin\varphi_i\;T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_i\right)\,. \tag{4.58}$$

The particles can no longer interact in the asymptotic range ($r_i \to \infty$ and $R_i \to \infty$) of the break-up channel and the total energy is split in a certain ration r_i/R_i into the two relative motions. Definite values for the lengths r_i and R_i fix ρ and the angle φ_i (via Eq. (4.15)), which determines the wavenumber $k_i = \sqrt{2\mu_{jk}E}\cos\varphi_i$ and via the relations between the different sets of Jacobi coordinates (Eqs. (4.21) and (4.22)) also $k_j = \sqrt{2\mu_{ik}E}\cos\varphi_j$ with $j \neq i$. The function $T_i(k)$ gives a spectrum of the partition of energy into the two relative motions. We proceed in calculating the break-up amplitude of the Faddeev component i,

$$\begin{aligned}
\psi_i(r_i, R_i) = \frac{u_i(r_i,R_i)}{r_iR_i} &\underset{\rho\to\infty}{\backsimeq} 2\mu_{i(jk)}\sqrt{2\mu_{jk}}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}}\sin\varphi_i\frac{1}{r_iR_i}T_i(k_i)\\
&= 2\mu_{i(jk)}\sqrt{2\mu_{jk}}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{1/2}}\sin\varphi_i\sqrt{2\mu_{i(jk)}}\sqrt{2\mu_{jk}}\frac{1}{\rho\sin\varphi_i}\frac{1}{\rho\underbrace{\cos\varphi_i}_{=\cos\left(\frac{\pi}{2}-\vartheta_i\right)}}T_i(k_i)\\
&= \left(2\mu_{i(jk)}\right)^{3/2}2\mu_{jk}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\frac{T_i(k_i)}{\sin\vartheta_i}\\
&= \left(2\mu_{i(jk)}\right)^{3/2}2\mu_{jk}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\frac{\sqrt{2\mu_{jk}E}}{k_i}T_i(k_i)\\
&= \left(4\mu_{i(jk)}\mu_{jk}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{3/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\frac{T_i(k_i)}{k_i}\,.
\end{aligned} \tag{4.59}$$

We used the transformation (4.47) and (4.53) and the saddle point condition $\vartheta_i = \frac{\pi}{2} - \varphi_i$, resulting from the integration along the line of steepest descent. The total wave function for the break-up channel is obtained by coherently summing up the three (different) Faddeev components, $\psi_i(r_i, R_i)$,

$$\Psi^{(+)}_{break-up} = \sum_{i=1}^{3}\psi_i(r_i, R_i) \underset{\substack{r_i\to\infty\\R_i\to\infty}}{\backsimeq} \sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{3/4}\frac{\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^{5/2}}\sum_{i=1}^{3}\left(4\mu_{i(jk)}\mu_{jk}\right)^{3/2}\frac{T_i(k_i)}{k_i} \tag{4.60}$$

4.2 Interior region and basis states for R-matrix formalism

We define an interior and exterior region that are separated by the boarder lines

$$\begin{aligned}
C_1:\; R_i = A_i \quad &\text{and} \quad 0 \le r_i \le a_i\\
C_2:\; r_i = a_i \quad &\text{and} \quad 0 \le R_i \le A_i\,.
\end{aligned} \tag{4.61}$$

The set of all points with $r_i \geq 0$ and $R_i \geq 0$ that are located inside that area is called D and we choose $r_i, R_i \in D$. We want to find values for the boundary parameters a_i and A_i that confine r_j, R_j ($j \neq i$) to D as well. The potential $V_i(r_i)$ occurs on the right hand side of Eq. (3.44) and has a maximum

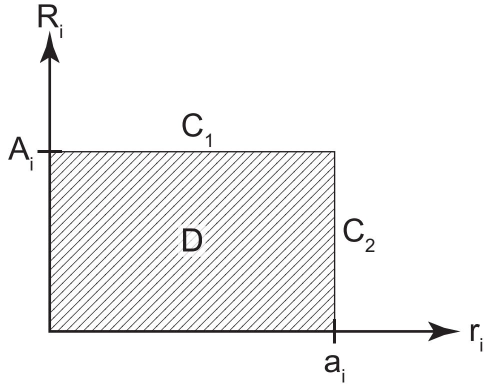

Figure 7: Interior region D with boundary lines C_1 and C_2.

range of r_{0i}. This value is used for r_i in the Jacobi relations (4.21) and (4.22), which then determine $r_{j_{max}}$, $R_{j_{max}}$. We use an upper bound approximation for the magnitudes r_j, R_j,

$$|a\mathbf{r}_i \pm b\mathbf{R}_i| = \sqrt{(ar_i)^2 \pm 2ab(\mathbf{r}_i \cdot \mathbf{R}_i) + (bR_i)^2} \approx \sqrt{(ar_i)^2 + 2abr_iR_i + (bR_i)^2} = ar_i + bR_i \,, \quad (4.62)$$

which makes it redundant to discriminate between the cases $i = 1, 2$ and $i = 3$ for the determination of the boundary parameters. Hence,

$$\begin{aligned} &\text{a)}\ \ \mathbf{r}_j = -\frac{m_j}{m_j+m_k}\mathbf{r}_i - (-1)^j\mathbf{R}_i \underset{r_j \text{ in } D}{\longrightarrow} \frac{m_j}{m_j+m_k}r_{0i} + A_i \leq a_i \\ &\text{b)}\, \mathbf{R}_j = (-1)^j \frac{m_im_k + m_jm_k + m_km_k}{(m_i+m_k)(m_j+m_k)}\mathbf{r}_i - \frac{m_i}{m_i+m_k}\mathbf{R}_i \underset{R_j \text{ in } D}{\longrightarrow} \\ &\frac{m_im_k + m_jm_k + m_km_k}{(m_i+m_k)(m_j+m_k)}r_{0i} + \frac{m_i}{m_i+m_k}A_i \leq A_i \end{aligned} \quad (4.63)$$

Expressing A explicitly from relation b) we get (with $\delta > 0$)

$$\text{b)}\ A_i \geq \frac{m_im_k + m_jm_k + m_km_k}{(m_j+m_k)m_k}r_{0i} = \frac{m_i+m_j+m_k}{(m_j+m_k)}r_{0i} \ \Rightarrow\ A_i = \frac{m_i+m_j+m_k}{(m_j+m_k)}r_{0i} + \delta \quad (4.64)$$

Inserting b) in a) gives

$$\text{a)}\ \frac{m_j}{m_j+m_k}r_{0i} + \frac{m_i+m_j+m_k}{(m_j+m_k)}r_{0i} \leq a_i \Rightarrow a_i \geq \frac{m_i+2m_j+m_k}{(m_j+m_k)}r_{0i} \Rightarrow a_i = \frac{m_i+2m_j+m_k}{(m_j+m_k)}r_0 + \delta \quad (4.65)$$

Thus, by choosing the boundary parameters,

$$\begin{aligned} a_i &= \sup_{j\neq i}\left\{\frac{m_i+2m_j+m_k}{m_j+m_k} r_{0i}\right\}+\delta\,, \\ A_i &= \frac{m_i+m_j+m_k}{m_j+m_k} r_{0i}+\delta\,, \end{aligned} \tag{4.66}$$

r_j, R_j are confined to D. The value of δ is chosen to be large enough for the asymptotic forms of $u_i(r_i, R_i)$, Eq. (4.37) and Eq.(4.45) to be valid on the lines C_1 and C_2. In the interior region D we expand the three Faddeev components $u_i(r_i, R_i)$ over a complete sets of basis states,

$$u_i(r_i, R_i) = \sum_\mu c_\mu^{(i)} \varphi_\mu(r_i, R_i)\,. \tag{4.67}$$

Each Faddeev component is therefore characterized by a certain set of expansion coefficients $c_\mu^{(i)}$, whereas the functions $\varphi_\mu(r_i, R_i)$ remain the same for all $u_i(r_i, R_i)$. These basis states $\varphi_\mu(r_i, R_i)$ obey the equation

$$\left[-\frac{1}{2\mu_{jk}}\frac{\mathrm{d}^2}{\mathrm{d}r_i^2} + V_i(r_i) - \frac{1}{2\mu_{i(jk)}}\frac{\mathrm{d}^2}{\mathrm{d}R_i^2} - E_\mu^{(i)}\right]\varphi_\mu(r_i, R_i) = 0\,, \tag{4.68}$$

with the boundary conditions

$$\varphi_\mu(0, R_i) = \varphi_\mu(r_i, 0) = \left.\frac{\varphi_\mu(r_i, R_i)}{\partial r_i}\right|_{r_i=a_i} = \left.\frac{\partial\varphi_\mu(r_i, R_i)}{\partial R_i}\right|_{R_i=A_i} = 0\,, \tag{4.69}$$

and are chosen to be real and orthonormal,

$$\iint_D \mathrm{d}r\,\mathrm{d}R\; \varphi_\mu(r, R)\varphi_{\mu'}(r, R) = \delta_{\mu\mu'}\,. \tag{4.70}$$

Thus, the expansion coefficients can be calculated as

$$c_\mu^{(i)} = \iint_D \mathrm{d}r\,\mathrm{d}R\; \varphi_\mu(r, R) u_i(r, R)\,. \tag{4.71}$$

In analogy to the case of three identical particles (Subsection 3.2.2) the introduced basis states $\varphi_\mu(r, R)$ can be chosen as product states

$$\varphi_\mu(r, R) = X_{\mu_1}(r) Y_{\mu_2}(R)\,, \tag{4.72}$$

where the functions $X_{\mu_1}(r)$ and $Y_{\mu_2}(R)$ are solutions to the equations

$$\left[-\frac{1}{2\mu_{jk}}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_i(r) - \epsilon_{\mu_1}^{(i)}\right] X_{\mu_1}(r) = 0 \tag{4.73}$$

and

$$\left[-\frac{1}{2\mu_{i(jk)}}\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \epsilon_{\mu_2}^{(i)}\right] Y_{\mu_2}(R) = 0\,. \tag{4.74}$$

The total energy $E_\mu^{(i)}$ is split into the energy of the two relative motions, $\epsilon_{\mu_1}^{(i)}$ (particle j relative to particle k) and $\epsilon_{\mu_2}^{(i)}$ (particle i relative to particle j and k). The set $\mu = \mu_1, \mu_2$ is arranged in that way that the total energy $E_\mu^{(i)} = \epsilon_{\mu_1}^{(i)} + \epsilon_{\mu_2}^{(i)}$ is approximately constant [6].

4.3 Equations for three-body R-matrix theory for arbitrary particle masses

We want to derive a set of equations that determine both, the expansion coefficients $c_\mu^{(i)}$ and consequently the wave functions in the interior region D and the on-shell T-matrix elements. First, we multiply both sides of Eq. (4.14) from the left with $\varphi_\mu(r_i, R_i)$,

$$\begin{aligned} &\varphi_\mu(r_i,R_i)\left[-\frac{1}{2\mu_{jk}}\frac{\mathrm{d}^2}{\mathrm{d}r_i^2} + V_i(r_i) - \frac{1}{2\mu_{i(jk)}}\frac{\mathrm{d}^2}{\mathrm{d}R_i^2} - E\right] u_i(r_i,R_i) = \\ &-\varphi_\mu(r_i,R_i)V_i(r_i)\int\limits_{-1}^{1}\mathrm{d}x_i\,\frac{r_iR_i}{2}\sum_{\substack{j=1\\j\neq i}}^{3}\frac{u_j(r_j,R_j)}{r_jR_j} \end{aligned} \tag{4.75}$$

and then integrate over the domain D,

$$\begin{aligned} &\iint_D \mathrm{d}r\,\mathrm{d}R\;\varphi_\mu(r_i,R_i)\left[-\frac{1}{2\mu_{jk}}\frac{\mathrm{d}^2}{\mathrm{d}r_i^2} + V_i(r_i) - \frac{1}{2\mu_{i(jk)}}\frac{\mathrm{d}^2}{\mathrm{d}R_i^2} - E\right] u_i(r_i,R_i) = \\ &-\iint_D \mathrm{d}r\,\mathrm{d}R\;\varphi_\mu(r_i,R_i)V_i(r_i)\int\limits_{-1}^{1}\mathrm{d}x_i\,\frac{r_iR_i}{2}\sum_{\substack{j=1\\j\neq i}}^{3}\frac{u_j(r_j,R_j)}{r_jR_j}\,. \end{aligned} \tag{4.76}$$

For the left hand side of Eq. (4.75) we can apply the results from Appendix E since the terms differ from those in Eq. (3.103) only in factors resulting from the different reduced masses,

$$(E_\mu^{(i)} - E)c_\mu^{(i)} - \frac{1}{2\mu_{i(jk)}}\int\limits_0^{a_i}\mathrm{d}r\;\varphi_\mu(r,A_i)\left.\frac{\mathrm{d}u_i}{\mathrm{d}R}\right|_{R=A_i} - \frac{1}{2\mu_{jk}}\int\limits_0^{A_i}\mathrm{d}R\;\varphi_\mu(a_i,R)\left.\frac{\mathrm{d}u_i}{\mathrm{d}r}\right|_{r=a_i}, \tag{4.77}$$

where $c_\mu^{(i)}$ and $E_\mu^{(i)}$ originate from Eqs. (4.71) and (4.68).

The right hand side of Eq. (4.76) reads

$$\begin{aligned} &-\iint_D \mathrm{d}r_i\mathrm{d}R_i\;\varphi_\mu(r_i,R_i)V_i(r_i)\int\limits_{-1}^{1}\mathrm{d}x_i\,\frac{r_iR_i}{2}\sum_{\substack{j=1\\j\neq i}}^{3}\frac{u_j(r_j,R_j)}{r_jR_j} \\ &= -\iint_D \mathrm{d}r_i\mathrm{d}R_i\;\varphi_\mu(r_i,R_i)V_i(r_i)\int\limits_{-1}^{1}\mathrm{d}x_i\,\frac{r_iR_i}{2}\sum_{\substack{j=1\\j\neq i}}^{3}\sum_{\mu'}\frac{c_{\mu'}^{(j)}\varphi_{\mu'}^{(j)}(r_j,R_j)}{r_jR_j}\,. \end{aligned} \tag{4.78}$$

The expansion of $u_j(r_j, R_j)$ in the source term is valid since r_j and R_j are located inside D, which is ensured by the values (4.66) for the boarder parameters A_i and a_i. With the matrix element

$$V_{\mu\mu'}^{(ij)} = \iint_D \mathrm{d}r_i \mathrm{d}R_i \ \varphi_\mu(r_i, R_i) V_i(r_i) \int\limits_{-1}^{1} \mathrm{d}x_i \ r_i R_i \frac{\varphi_{\mu'}(r_j, R_j)}{2 r_j R_j} \,, \tag{4.79}$$

Eq. (4.76) finally becomes

$$(E_\mu^{(i)} - E) c_\mu^{(i)} + \sum_{\mu'} \sum_{\substack{j=1 \\ j \neq i}}^{3} V_{\mu\mu'}^{(ij)} c_{\mu'}^{(j)} = \frac{1}{2\mu_{i(jk)}} \int\limits_0^{a_i} \mathrm{d}r \ \varphi_\mu(r, A_i) \left. \frac{\mathrm{d}u_i}{\mathrm{d}R} \right|_{R=A_i} + \frac{1}{2\mu_{jk}} \int\limits_0^{A_i} \mathrm{d}R \ \varphi_\mu(a_i, R) \left. \frac{\mathrm{d}u_i}{\mathrm{d}r} \right|_{r=a_i} . \tag{4.80}$$

The index "i" in $V_{\mu\mu'}^{(ij)}$ indicates the potential that occurs in the matrix element. Inserting the asymptotic forms (4.37) and (4.45) on the boarder lines C_1 and C_2 into the right hand side of Eq. (4.80) yields

$$\begin{aligned}
&(E_\mu - E) c_\mu^{(i)} + \sum_{\mu'} \sum_{\substack{j=1 \\ j \neq i}}^{3} V_{\mu\mu'}^{(ij)} c_{\mu'}^{(j)} \\
=& \frac{1}{2\mu_{i(jk)}} \int\limits_0^{a_i} \mathrm{d}r \ \varphi_\mu(r, A_i) u_i^b(r) Q \cos(Q A_i) - \int\limits_0^{a_i} \mathrm{d}r \ \varphi_\mu(r, A_i) u_i^b(r) \mathrm{i} Q \mathrm{e}^{\mathrm{i} Q A_i} T_i^b \\
&- \frac{2}{\pi} \int\limits_0^{a_i} \mathrm{d}r \ \varphi_\mu(r, A_i) \int\limits_0^{\sqrt{2\mu_{jk} E}} \mathrm{d}k \ u_k^{(-)}(r) \mathrm{i} Q_k \mathrm{e}^{\mathrm{i} Q_k A_i} T_i(k) \\
&- \sum_{\substack{j=1 \\ j \neq i}}^{3} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)} E} \frac{m_i}{m_i + m_k} R_i / \sin\varphi_j^*}}{R_i^{3/2}} \mathrm{i} \sqrt{2\mu_{j(ik)} E} \frac{m_i}{m_i + m_k} / \sin\varphi_j^* \\
&\times \left(\int\limits_0^{a_i} \mathrm{d}r \ \varphi_\mu(r, A_i) u_i^b(r) C_i^b + \int\limits_0^{a_i} \mathrm{d}r \ \varphi_\mu(r, A_i) \int\limits_{\sqrt{2\mu_{jk} E}}^{\infty} \mathrm{d}k \ u_k^{(-)}(r) C_i(k) \right) \\
&- \frac{2\mu_{i(jk)}}{\pi \mu_{jk}} \int\limits_0^{A_i} \mathrm{d}R \ \varphi_\mu(a_i, R) \int\limits_0^{\sqrt{2\mu_{jk} E}} \mathrm{d}k \ \sin(Q_k R) \mathrm{i} k \mathrm{e}^{\mathrm{i} k a_i} T_i(k)
\end{aligned} \tag{4.81}$$

Terms of the order $R^{-\alpha}$ with $\alpha > 3/2$ were neglected. We can replace the numbers C in Eq. (4.81) by T-matrix elements, respectively. Comparing Eqs. (4.58) and (4.16) reveals that the function A is somehow related to $T(k)$,

$$\mathrm{A}(\varphi_i^*) = 2\mu_{i(jk)} \sqrt{2\mu_{jk}} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \sin\varphi_i^* \ T_i\left(\sqrt{2\mu_{jk} E} \cos\varphi_i^* \right) . \tag{4.82}$$

Consequently,

$$
\begin{aligned}
C_i^b =& \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} 2\mu_{i(jk)} \sqrt{2\mu_{jk}} (2\mu_{j(ik)})^{-1/4} \left(\frac{m_i+m_k}{m_i}\right)^{5/2} (\sin\varphi_j^*)^{7/2} E^{1/4} T_i \left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right) \\
& \times \frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E - \frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)} \int\limits_0^\infty \mathrm{d}r \; u_i^b(r) V_i(r) \,,
\end{aligned} \tag{4.83}
$$

and

$$
\begin{aligned}
C_i(k) =& \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} 2\mu_{i(jk)} \sqrt{2\mu_{jk}} \left(2\mu_{j(ik)}\right)^{-1/4} \left(\frac{m_i+m_k}{m_i}\sin\varphi_j^*\right)^{3/2} E^{1/4} T_i \left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right) \\
& \times \frac{1}{\frac{1}{\mu_{jk}}k^2 - 2E + 2\frac{\mu_{j(ik)}}{\mu_{i(jk)}} E \left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2} \int\limits_0^\infty \mathrm{d}r \; u_k^{(-)*}(r) V_i(r) \,.
\end{aligned} \tag{4.84}
$$

Using these results for the numbers C and the shortcuts

$$
\begin{aligned}
M_{\mu b} &= \int\limits_0^{a_i} \mathrm{d}r \; \varphi_\mu(r, A_i) u_i^b(r) \\
M_{\mu k}^{(-)} &= \int\limits_0^{a_i} \mathrm{d}r \; \varphi_\mu(r, A_i) u_k^{(-)}(r) \\
M_{\mu Q} &= \int\limits_0^{A_i} \mathrm{d}R \; \varphi_\mu(a_i, R) \sin(QR) \,,
\end{aligned} \tag{4.85}
$$

Eq. (4.81) turns into

$$
\begin{aligned}
&(E_\mu - E)c_\mu^{(i)} + \sum_{\substack{j=1\\ j\neq i}}^{3}\sum_{\mu'} V_{\mu\mu'}^{(j)} c_{\mu'}^{(j)} \equiv \sum_{\substack{j=1\\ j\neq i}}^{3}\sum_{\mu'} R_{\mu\mu'}(E) c_{\mu'}^{(j)} = \frac{1}{2\mu_{i(jk)}} Q M_{\mu b}\cos(QA_i) - \mathrm{i}QM_{\mu b}\mathrm{e}^{\mathrm{i}QA_i}T_i^b \\
&-\frac{2}{\pi}\int_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k\ \mathrm{i}Q_k M_{\mu k}^{(-)} \mathrm{e}^{\mathrm{i}Q_k A_i} T_i(k) \\
&-\frac{1}{2\mu_{i(jk)}}\sum_{\substack{j=1\\ j\neq i}}^{3} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} \mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}/\sin\varphi_j^* \\
&\times\Bigg(\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}} 2\mu_{i(jk)}\sqrt{2\mu_{jk}}(2\mu_{j(ik)})^{-\frac{1}{4}}\left(\frac{m_i+m_k}{m_i}\right)^{\frac{5}{2}} (\sin\varphi_j^*)^{\frac{7}{2}} E^{\frac{1}{4}} M_{\mu b} T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right) \\
&\quad\times\frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E - \frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)}\int_0^{r_{0i}} \mathrm{d}r\ u_i^b(r)V_i(r) \\
&\quad+\left(\frac{2}{\pi}\right)^{\frac{3}{2}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} 2\mu_{i(jk)}\sqrt{2\mu_{jk}}\left(2\mu_{j(ik)}\right)^{-\frac{1}{4}}\left(\frac{m_i+m_k}{m_i}\sin\varphi_j^*\right)^{\frac{3}{2}} E^{\frac{1}{4}} \\
&\quad\times\int_{\sqrt{2\mu_{jk}E}}^{\infty} \mathrm{d}\ k M_{\mu k}^{(-)} T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right)\frac{1}{\frac{1}{\mu_{jk}}k^2 - 2E + 2\frac{\mu_{j(ik)}}{\mu_{i(jk)}}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2} \\
&\quad\times\int_0^{\infty}\mathrm{d}r\ u_k^{(-)*}(r)V_i(r)\Bigg) - \frac{2\mu_{i(jk)}}{\pi\mu_{jk}}\int_0^{\sqrt{2\mu_{jk}E}}\mathrm{d}k\ \mathrm{i}kM_{\mu Q_k}\mathrm{e}^{\mathrm{i}ka_i}T_i(k) \\
=&\frac{1}{2\mu_{i(jk)}}QM_{\mu b}\cos(QA_i) - \mathrm{i}QM_{\mu b}\mathrm{e}^{\mathrm{i}QA_i}T_i^b \\
&-\frac{2}{\pi}\int_0^{\sqrt{2\mu_{jk}E}}\mathrm{d}k\left[\mathrm{i}Q_kM_{\mu k}^{(-)}\mathrm{e}^{\mathrm{i}Q_kA_i} + \frac{\mu_{i(jk)}}{\mu_{jk}}\mathrm{i}kM_{\mu Q_k}\mathrm{e}^{\mathrm{i}ka_i}\right]T_i(k) \\
&-\sum_{\substack{j=1\\ j\neq i}}^{3}\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right) \\
&\times\Bigg(N_b(E)M_{\mu b}\frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E-\frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)}\int_0^{r_{0i}}\mathrm{d}r\ u_i^b(r)V_i(r) \\
&\quad+\frac{2}{\pi}N_k(E)\int_{\sqrt{2\mu_{jk}E}}^{\infty} M_{\mu k}^{(-)}\frac{1}{\frac{1}{\mu_{jk}}k^2 - 2E + 2\frac{\mu_{j(ik)}}{\mu_{i(jk)}}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\int_0^{\infty}\mathrm{d}r\ u_k^{(-)*}(r)V_i(r)\Bigg),
\end{aligned}
\tag{4.86}
$$

with

$$N_b(E) = \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} \sqrt{2\mu_{jk}} (2\mu_{j(ik)})^{\frac{1}{4}} \left(\frac{m_i + m_k}{m_i}\right)^{\frac{3}{2}} (\sin\varphi_j^*)^{\frac{5}{2}} E^{\frac{3}{4}} , \tag{4.87}$$

and

$$N_k(E) = \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} 2\mu_{i(jk)} \sqrt{2\mu_{jk}} \left(2\mu_{j(ik)}\right)^{\frac{1}{4}} \left(\frac{m_i + m_k}{m_i} \sin\varphi_j^*\right)^{\frac{1}{2}} E^{\frac{3}{4}} . \tag{4.88}$$

We define the three-particle R-matrix for arbitrary particle masses according to

$$R_{\mu\mu'}(E) = \delta_{ij}\delta_{\mu\mu'}(E_\mu - E) + V_{\mu\mu'}^{(j)} . \tag{4.89}$$

which is the matrix representation of the Faddeev equations inside the region D. Thus, Eq. (4.86) relates the Faddeev equations in matrix form inside the domain D on the left hand side with the logarithmic derivatives of the asymptotic wavefunction $u_i(r_i, R_i)$ on the boundary lines C_1 and C_2 on the right hand side. It is the first of a set of four equations in R-matrix theory to calculate the expansion coefficients $c_\mu^{(i)}$ and the T-matrix elements T_i^b and $T_i(k)$.

The remaining three equations arise from equating the interior and exterior wave functions on the two boundary lines C_1 and C_2, respectively. Initially, we will ignore terms of the order $R^{-3/2}$ occurring in the asymptotic form (4.37) of u_i. However, later they can be considered in order to improve the accuracy of the results.

Proceeding from Eq. (4.37), we expand the wave function $u_i(r_i, R_i)$ *inside* the region D on the left hand side in basis functions $\varphi_\mu(r, R)$. On the right hand side, we have its asymptotic form *outside* D. On the line C_1 with $R = A_i$ we require the interior and exterior wave function to be equal, which after projecting onto the (real) binding wave function u_i^b, leads to

$$\begin{aligned}\int_0^{a_i} \mathrm{d}r\; u_b^i(r) \sum_\mu c_\mu^{(i)} \varphi_\mu(r, A_i) \backsimeq & \underbrace{\int_0^{a_i} \mathrm{d}r\; \left|u_b^i(r)\right|^2}_{=1} \sin(QA_i) - 2\mu_{i(jk)} \underbrace{\int_0^{a_i} \mathrm{d}r\; \left|u_b^i(r)\right|^2}_{=1} \mathrm{e}^{\mathrm{i}QA_i} T_i^b \\ & - \frac{4}{\pi}\mu_{i(jk)} \int_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \underbrace{\int_0^{a_i} \mathrm{d}r\; u_b^i(r) u_k^{(-)}(r)}_{\approx 0} \mathrm{e}^{\mathrm{i}Q_k A_i} T_i(k) ,\end{aligned} \tag{4.90}$$

where we used orthonormality of the bound states u_i^b and approximated $\int_0^{a_i} \mathrm{d}r\; u_b(r) u_k^{(-)}(r) \approx 0$ on the line C_1. Latter is justified since the bound states are spatially localized and therefore $u_b(a_i) \approx 0$ on the line C_2 with sufficiently large a_i. This approximation has already been used when deriving the asymptotic form (4.58) in the break-up channel from Eq. (4.37). Including Eq. (4.85) yields the final form

$$\sum_\mu M_{\mu b} c_\mu^{(i)} \backsimeq \sin(QA_i) - 2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}QA_i} T_i^b , \tag{4.91}$$

which connects $c_\mu^{(i)}$ with the T-matrix elements T_i^b. Once more we start with the asymptotic form of $u_i(r_i, R_i)$ in the limit $R_i \to \infty$ and r_i fixed (without terms $\sim R^{-3/2}$),

$$u_i(r_i, R_i) \backsimeq u_i^b(r_i)\sin(QR_i) - 2\mu_{i(jk)} u_i^b(r_i) \mathrm{e}^{\mathrm{i}QR_i} T_i^b - \frac{4}{\pi}\mu_{i(jk)} \int\limits_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k\; u_k^{(-)}(r_i)\mathrm{e}^{\mathrm{i}Q_kR_i} T_i(k)\,,$$

and now replace the integral by its asymptotic expansion (4.58). Then, on the line C_1, where the interior and exterior wave functions are set to be equal, we get

$$\begin{aligned}&\sum_\mu c_\mu^{(i)} \varphi_\mu(r_i, A_i) - u_i^b(r_i)\left[\sin(QA_i) - 2\mu_{i(jk)}\mathrm{e}^{\mathrm{i}QA_i}T_i^b\right] \\ &\backsimeq (2\mu_{i(jk)})^{3/2}\sqrt{2\mu_{jk}}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho_A\sqrt{E}}}{\rho_A^{1/2}}\frac{A_i}{\rho_A}\;T_i\left(2\mu_{jk}\sqrt{E}\frac{r_i}{\rho_A}\right)\,,\end{aligned} \tag{4.92}$$

with $\rho_A = \sqrt{2\mu_{jk}r_i^2 + 2\mu_{i(jk)}A_i^2}$ and $\sin\varphi_i|_{C_1} = \sqrt{2\mu_{i(jk)}}\dfrac{A_i}{\rho_A}$. The same procedure is carried out on the line C_2 and provides the fourth equation,

$$\begin{aligned}&\sum_\mu c_\mu^{(i)} \varphi_\mu(a_i, R_i) \\ &\backsimeq u_i^b(a_i)\left[\sin(QR_i) - \mathrm{e}^{\mathrm{i}QR_i}T_i^b\right] + \left(2\mu_{i(jk)}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho_a\sqrt{E}}}{\rho_a^{1/2}}\frac{R_i}{\rho_a}\;T_i\left(2\mu_{jk}\sqrt{E}\frac{a_i}{\rho_a}\right) \\ &\backsimeq \left(2\mu_{i(jk)}\right)^{3/2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}E^{1/4}\frac{\mathrm{e}^{\mathrm{i}\rho_a\sqrt{E}}}{\rho_a^{1/2}}\frac{R_i}{\rho_a}\;T_i\left(2\mu_{jk}\sqrt{E}\frac{a_i}{\rho_a}\right)\,,\end{aligned} \tag{4.93}$$

with $\rho_a = \sqrt{2\mu_{jk}a_i^2 + 2\mu_{i(jk)}R_i^2}$ and $u_i^b(a_i) \approx 0$. Hence, we have found a set of four equations for channel α,

$$
\begin{aligned}
&1)(E_\mu - E)c_\mu^{(i)} + \sum_{\substack{j=1\\ j\neq i}}^{3} \sum_{\mu'} V_{\mu\mu'}^{(j)} c_{\mu'}^{(j)} \\
&\quad = \frac{1}{2\mu_{i(jk)}} Q M_{\mu b} \cos(QA_i) - \mathrm{i} Q M_{\mu b} \mathrm{e}^{\mathrm{i}QA_i} T_i^b \\
&\quad - \frac{2}{\pi} \int\limits_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \left[\mathrm{i} Q_k M_{\mu k}^{(-)} \mathrm{e}^{\mathrm{i}Q_k A_i} + \frac{\mu_{i(jk)}}{\mu_{jk}} \mathrm{i}k M_{\mu Q_k} \mathrm{e}^{\mathrm{i}k a_i} \right] T_i(k) \\
&\quad - \sum_{\substack{j=1\\ j\neq i}}^{3} \frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i / \sin\varphi_j^*}}{R_i^{3/2}} T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right) \\
&\times \left(N_b(E) M_{\mu b} \frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E - \frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)} \int\limits_0^{r_{0i}} \mathrm{d}r\; u_i^b(r) V_i(r) \right. \\
&\quad \left. + \frac{2}{\pi} N_k(E) \int\limits_{\sqrt{2\mu_{jk}E}}^{\infty} \mathrm{d}k\; M_{\mu k}^{(-)} \frac{1}{\frac{1}{\mu_{jk}}k^2 - 2E + 2\frac{\mu_{j(ik)}}{\mu_{i(jk)}} E \left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2} \int\limits_0^{r_{0i}} \mathrm{d}r\; u_k^{(-)*}(r) V_i(r) \right) \\
&2) \sum_\mu M_{\mu b} c_\mu^{(i)} \simeq \sin(QA_i) - 2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}QA_i} T_i^b \\
&3) \sum_\mu c_\mu^{(i)} \varphi_\mu(r_i, A_i) - u_i^b(r_i) \left[\sin(QA_i) - 2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}QA_i} T_i^b\right] \\
&\quad \simeq (2\mu_{i(jk)})^{3/2} \sqrt{2\mu_{jk}} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho_A\sqrt{E}}}{\rho_A^{1/2}} \frac{A_i}{\rho_A}\; T_i\left(2\mu_{jk}\sqrt{E}\frac{r_i}{\rho_A}\right) \\
&4) \sum_\mu c_\mu^{(i)} \varphi_\mu(a_i, R_i) \simeq \left(\frac{4}{3}\right)^{3/2} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho_a\sqrt{E}}}{\rho_a^{1/2}} \frac{R}{\rho_a}\; T_i\left(\sqrt{E}\frac{a}{\rho_a}\right),
\end{aligned}
\tag{4.94}
$$

It determines the expansion coefficients $c_\mu^{(i)}$ and the T-matrix elements T_i^b for the bound states and $T_i(k)$ for the scattering states. By solving this system of equations we can calculate the cross section and the wave function inside the area D. Again, in low energy regions, there occur some simplifications, which have already been discussed in Sec. 3.2.3.

5 Conclusion

W. Glöckle has established a R-matrix method for three-particle channels on the basis of Faddeev equations. He has found a set of four equations (3.122) that allows us to calculate the expansion coefficients of the interior wave functions and the T-matrix elements. In this thesis we extended the three body R-matrix method to three arbitrary particle masses and finally obtained a similar set of equations (4.94).

In our formalism we can describe all reactions (except for a three-particle bound state) that take place when a projectile hits a two-particle bound state. In Subsection 3.2.4, we found that the total asymptotic behavior of the wave function in a certain channel (except for the break-up and the three-particle bound channel) is contained in the Faddeev component corresponding to that channel. Hence, for instance in channel α, the cross section for elastic scattering is obtained by calculating the amplitude T_b^i with $i = \alpha$ and for rearrangement processes via the amplitude T_b^i with $i = \beta$ or $i = \gamma$. The cross section for break-up reactions is the coherent sum over the squared matrix elements $T_i(k)$. This shows that contributions to the break-up channel arise from all three Faddeev components. A theoretically existing fifth channel where all particle stick together and form one bound state has been neglected.

For the (numerical) solution of the set (4.94) one has to note that for three arbitrary particles the equations are coupled. That means that one Faddeev component depends on the others via the T-amplitudes that contain a source term Q_i. In (3.122) this is different, since for three identical particles the number of Faddeev components reduce from three to one. Methods of solution have not yet been established, but will follow in the near future.

Appendix

A Verification of Eq. (3.48)

We want to show that the asymptotic form (3.47) of the wave function $u(\rho,\varphi)$ satisfies Eq. (3.48),

$$
\begin{aligned}
&\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}-\frac{1}{\rho^2}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}-E\right]\left(\frac{\mathrm{e}^{i\sqrt{E}\rho}}{\rho^{1/2}}\mathrm{A}(\varphi)\right)= \\
&-\frac{\mathrm{e}^{i\sqrt{E}\rho}}{\rho^2}\mathrm{A}(\varphi)\left[i\sqrt{E}\left(i\sqrt{E}\rho^{1/2}-\frac{1}{2}\rho^{-1/2}\right)\rho+\left(\frac{1}{2}i\sqrt{E}\rho^{-1/2}+\frac{1}{4}\rho^{-3/2}\right)\rho-\left(i\sqrt{E}\rho^{1/2}-\frac{1}{2\rho^{-1/2}}\right)\right] \\
&-\frac{\mathrm{e}^{i\sqrt{E}\rho}}{\rho}\mathrm{A}(\varphi)\left(i\sqrt{E}\rho^{1/2}-\frac{1}{2}\rho^{-1/2}\right)-\frac{1}{\rho^2}\frac{\mathrm{d}^2\mathrm{A}(\varphi)}{\mathrm{d}\varphi^2}-E\frac{\mathrm{e}^{i\sqrt{E}\rho}}{\rho^{1/2}}\mathrm{A}(\varphi) \\
&=\mathrm{e}^{i\sqrt{E}\rho}\mathrm{A}(\varphi)\Big(E\rho^{-1/2}+\frac{1}{2}i\sqrt{E}\rho^{-3/2}-\frac{1}{2}i\sqrt{E}\rho^{-3/2}-\frac{1}{4}\rho^{-5/2}+i\sqrt{E}\rho^{-3/2}-\frac{1}{2}\rho^{-5/2} \\
&-i\sqrt{E}\rho^{-3/2}+\frac{1}{2}\rho^{-5/2}-E\rho^{-1/2}\Big)-\frac{1}{\rho^2}\frac{\mathrm{d}^2\mathrm{A}(\varphi)}{\mathrm{d}\varphi^2}=-\frac{\mathrm{e}^{i\sqrt{E}\rho}}{4\rho^{5/2}}\mathrm{A}(\varphi)-\frac{1}{\rho^2}\frac{\mathrm{d}^2\mathrm{A}(\varphi)}{\mathrm{d}\varphi^2}\underset{\rho\to\infty}{\longrightarrow}0\,.
\end{aligned}
\tag{A.1}
$$

In the case of three distinguishable particles the procedure remains the same. The asymptotic form of u from its functional form is the same as for identical particles, only the reduced masses change.

B Additional terms of asymptotic $u(r_1, R_1)$

Inserting the asymptotic form of the source term $Q(r_1, R_1)$ (Eq. (3.53)) into the first line of Eq. (3.57) and omitting non R_1'-dependent terms, yields

$$I = \frac{4}{3} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \frac{\sin[Q(R_1 - R_1')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \,. \tag{B.1}$$

We integrate by parts the first time and obtain

$$\begin{aligned} I =& \frac{4}{3Q} \left[\frac{1}{Q} \cos[Q(R_1 - R_1')] \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \right] \Bigg|_{R_1}^{\infty} - \frac{3}{4Q^2} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \cos[Q(R_1 - R_1')] \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'} \left(\mathrm{i}\sqrt{\frac{4}{3}E}R_1' - \frac{3}{2} \right)}{R_1'^{5/2}} \\ =& \frac{1}{\frac{3}{4}Q^2} \left[0 - \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}} \right] - \frac{1}{\frac{3}{4}Q^2} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \cos[Q(R_1 - R_1')] \frac{\mathrm{i}\sqrt{\frac{4}{3}E} \cdot \mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \,. \end{aligned} \tag{B.2}$$

The term proportional to $R_1^{'-5/2}$ in the second line of Eq. (B.2) is neglected in the following as it decreases faster to zero for $R_1 \to \infty$ than the others. Integrating the second term in Eq. (B.2) once more by parts

$$\begin{aligned} & - \frac{1}{\frac{3}{4}Q^2} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \cos[Q(R_1 - R_1')] \frac{\mathrm{i}\sqrt{\frac{4}{3}E} \cdot \mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \\ &= - \frac{1}{\frac{3}{4}Q^2} \left[- \frac{1}{Q} \sin[Q(R_1 - R_1')] \frac{\mathrm{i}\sqrt{\frac{4}{3}E} \cdot \mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \right] \Bigg|_{R_1}^{\infty} \\ & - \frac{1}{Q^2} \frac{4}{3} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \frac{\sin[Q(R_1 - R_1')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \left(-\frac{4}{3}E \right) \\ &= - \frac{1}{\frac{3}{4}Q^2} [0 - 0] + \frac{1}{Q^2} \frac{4}{3} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \frac{\sin[Q(R_1 - R_1')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \left(\frac{4}{3}E \right) \\ &= \frac{1}{Q^2} \left[\frac{4}{3} \int_{R_1}^{\infty} \mathrm{d}R_1' \; \frac{\sin[Q(R_1 - R_1')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \right] \left(\frac{4}{3}E \right) \end{aligned} \tag{B.3}$$

Thus, the integral we started with is reproduced and enables us to write down the solution

$$
\begin{aligned}
I &= -\frac{1}{\frac{3}{4}Q^2}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}} + \frac{1}{Q^2}I\frac{4}{3}E \\
I\cdot\left(1-\frac{1}{Q^2}\frac{4}{3}E\right) &= -\frac{1}{\frac{3}{4}Q^2}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}} \\
I\cdot\underbrace{\left(\frac{3}{4}Q^2-E\right)}_{=-E_b} &= -\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}} \\
I &= \frac{1}{E_b}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}
\end{aligned}
\tag{B.4}
$$

In the last equality of Eq. (B.4) we used $E_b = E - \frac{3}{4}Q^2$ following from Eq. (3.55). The total expression for the first additional term of the asymptotic form of $u(r_1, R_1)$ in the limit $R_1 \to \infty$ and r_1 fixed, reads

$$
H_1(R_1) = 4\left(\frac{3}{4}\right)^{1/4}\mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\frac{1}{E_b}\int_0^{r_0}\mathrm{d}r_1'\; r_1' u_b(r_1')V(r_1')\,. \tag{B.5}
$$

Next, we want to derive the second term $H_2(r_1, R_1)$ presented in Eq. (3.58). Because now the integration interval goes from $\sqrt{E}$ to infinity, from $E = k^2 + \frac{3}{4}Q_k^2$ it follows that Q_k must be a complex quantity. To be consistent with [6] we introduce the following notation,

$$
E = k^2 + \frac{3}{4}Q_k^2 \longrightarrow E = Q_K^2 - \frac{3}{4}K^2\,, \tag{B.6}
$$

with

$$
Q_k \hat{=} \mathrm{i}K \qquad \text{and} \qquad k \hat{=} Q_K \tag{B.7}
$$

where K, Q_K and k are real quantities. Differentiating the second relation in Eq. (B.6) leads to

$$
\begin{aligned}
2k\;\mathrm{d}k &= 2\frac{3}{4}K\mathrm{d}K \\
\mathrm{d}k &= \frac{3}{4}\cdot\frac{K}{k}\mathrm{d}K\,,
\end{aligned}
\tag{B.8}
$$

where we used $k \hat{=} Q_K$. So we can transform the integrals over k from Eq. (3.56),

$$
\begin{aligned}
&-\frac{4}{3}\cdot\frac{2}{\pi}\int_{\sqrt{E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_k R_1}\int_0^{R_1}\mathrm{d}R_1'\;\frac{\sin(Q_k R_1')}{Q_k}\int_0^{\infty}\mathrm{d}r_1'\; u_k^{(-)*}(r_1')V(r_1')Q(r_1', R_1') \\
&-\frac{4}{3}\cdot\frac{2}{\pi}\int_{\sqrt{E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_1)\frac{\sin(Q_k R_1')}{Q_k}\int_{R_1}^{\infty}\mathrm{d}R_1'\;\mathrm{e}^{\mathrm{i}Q_k R_1}\int_0^{\infty}\mathrm{d}r_1'\; u_k^{(-)*}(r_1')V(r_1')Q(r_1', R_1')\,,
\end{aligned}
\tag{B.9}
$$

into

$$
\begin{aligned}
H_2(r_1, R_1) = & -\frac{4}{3}\cdot\frac{2}{\pi}\int\limits_0^\infty \mathrm{d}K\ \frac{3}{4}\cdot\frac{K}{k}\cdot\frac{u^{(-)}_{Q_K}(r_1)}{\mathrm{i}K}\left[\mathrm{e}^{\mathrm{i}^2 KR_1}\int\limits_0^{R_1}\mathrm{d}R_1'\ \sin(\mathrm{i}KR_1') + \sin(\mathrm{i}KR_1)\int\limits_{R_1}^\infty \mathrm{d}R_1'\ \mathrm{e}^{\mathrm{i}^2 KR_1'}\right] \\
& \times \int\limits_0^{r_0}\mathrm{d}r_1'\ u^{(-)*}_{Q_K}(r_1')V(r_1')Q(r_1', R_1') \\
= & -\frac{2}{\pi}\int\limits_0^\infty \mathrm{d}K\ \frac{u^{(-)}_{Q_K}(r_1)}{\mathrm{i}k}\left[\mathrm{e}^{-KR_1}\int\limits_0^{R_1}\mathrm{d}R_1'\ \mathrm{i}\sinh(KR_1') + \mathrm{i}\sinh(KR_1)\int\limits_{R_1}^\infty \mathrm{d}R_1'\ \mathrm{e}^{-KR_1'}\right] \\
& \times \int\limits_0^{r_0}\mathrm{d}r_1'\ u^{(-)*}_{Q_K}(r_1')V(r_1')Q(r_1', R_1') \\
= & -\frac{2}{\pi}\int\limits_0^\infty \mathrm{d}K\ \frac{u^{(-)}_{Q_K}(r_1)}{Q_K}\left[\mathrm{e}^{-KR_1}\int\limits_0^{R_1}\mathrm{d}R_1'\ \sinh(KR_1') + \sinh(KR_1)\int\limits_{R_1}^\infty \mathrm{d}R_1'\ \mathrm{e}^{-KR_1'}\right] \\
& \times \int\limits_0^{r_0}\mathrm{d}r_1'\ u^{(-)*}_{Q_K}(r_1')V(r_1')Q(r_1', R_1')\,.
\end{aligned}
\tag{B.10}
$$

The integration over K is split according to $\int_0^\infty \mathrm{d}K = \int_0^{K_0(R_1)} \mathrm{d}K + \int_{K_0(R_1)}^\infty \mathrm{d}K$ with $K_0(R_1)\cdot R_1 \to \infty$ and $K_0(R_1) \to 0$ for $R_1 \to \infty$. For $K \geq K_0$ we carry out the integration over R_1' by parts and use the asymptotic form of $Q(r_1, R_1)$ from Eq. (3.53) (the R_1- dependent part only),

$$
\begin{aligned}
H_2^{(1)}(r_1, R_1) = & \sinh(KR_1)\int\limits_{R_1}^\infty \mathrm{d}R_1'\ \mathrm{e}^{-KR_1'}\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} = \frac{\sinh(KR_1)}{\mathrm{i}\sqrt{\frac{4}{3}E}-K}\cdot\left.\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'-KR_1'}}{R_1'^{3/2}}\right|_{R_1}^\infty + O\left(\frac{1}{R_1^{5/2}}\right) \\
\backsimeq & \ 0 - \frac{1}{2}\left(\mathrm{e}^{KR_1}-\mathrm{e}^{-KR_1}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1-KR_1}}{R_1^{3/2}\left(\mathrm{i}\sqrt{\frac{4}{3}E}-K\right)} = \frac{1}{2}\cdot\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}\left(K-\mathrm{i}\sqrt{\frac{4}{3}E}\right)} + O\left(\mathrm{e}^{-2K_0R_1}\right)
\end{aligned}
\tag{B.11}
$$

and

$$
\begin{aligned}
H_2^{(2)}(r_1, R_1) =& \mathrm{e}^{-KR_1} \int\limits_0^{R_1'} \mathrm{d}R_1' \, \frac{1}{2} \left(\mathrm{e}^{KR_1'} - \mathrm{e}^{-KR_1'} \right) \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \\
=& \frac{1}{2} \frac{\mathrm{e}^{-KR_1}}{K + \mathrm{i}\sqrt{\frac{4}{3}E}} \left[\frac{\mathrm{e}^{KR_1' + \mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} - \frac{\mathrm{e}^{-KR_1' + \mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \right] \Bigg|_0^{R_1} + O\left(\frac{1}{R_1^{5/2}} \right) \\
\backsimeq& \frac{1}{2} \frac{\mathrm{e}^{-KR_1}}{K + \mathrm{i}\sqrt{\frac{4}{3}E}} \frac{\mathrm{e}^{KR_1' + \mathrm{i}\sqrt{\frac{4}{3}E}R_1'}}{R_1'^{3/2}} \Bigg|_0^{R_1} + O\left(\mathrm{e}^{-2K_0 R_1} \right) \\
\backsimeq& \frac{1}{2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2} \left(K + \mathrm{i}\sqrt{\frac{4}{3}E} \right)} \, .
\end{aligned}
\tag{B.12}
$$

Terms of order $R_1^{-\alpha}$ with $\alpha > \frac{3}{2}$ are neglected in Eqs. (B.11) and (B.12). In Eq. (B.12) we put $\int\limits_0^{R_1} \mathrm{d}R_1' = \int\limits_0^{d} \mathrm{d}R_1' + \int\limits_d^{R_1} \mathrm{d}R_1'$, where d is such that the asymptotic form of $Q(r_1, R_1)$ can be applied. In the interval $0 \leq K \leq K_0$ we only keep the leading part of $H_2(r_1, R_1)$ which is

$$
\begin{aligned}
H_2^{(3)}(r_1, R_1) \backsimeq& -\frac{2}{\pi} \frac{u_{Q_0}^{(-)}(r_1)}{Q_0} \int\limits_0^{r_0} \mathrm{d}r_1' \, u_{Q_0}^{(-)*}(r_1') V(r_1') Q(r_1', R_1') \\
& \times \int\limits_0^{K_0} \mathrm{d}K \left[\mathrm{e}^{-KR_1} \int\limits_0^{R_1} \mathrm{d}R_1' \, \sinh(KR_1') + \sinh(KR_1) \int\limits_{R_1}^{\infty} \mathrm{d}R_1' \, \mathrm{e}^{-KR_1'} \right]
\end{aligned}
\tag{B.13}
$$

and can be estimated, according to [6], to be of the order $O\left(\frac{1}{R_1^2}\right)$ for $R_1 \to \infty$. Q_0, or more precisely Q_{K_0}, is independent of K and the greatest value of Q in the interval $0 \leq K \leq K_0$, thus it has to be considered in the leading term $H_2^{(3)}(r_1, R_1)$. The total term $H_2(r_1, R_1)$ is composed of $H_2^{(1)}, H_2^{(2)}$ and

$H_2^{(3)}$ and includes the total asymptotic form of Q,

$$\begin{aligned}
H_2(r_1,R_1) \backsimeq & -\frac{2}{\pi}\int\limits_{K_0}^{\infty} \mathrm{d}K\, \frac{u_{Q_K}^{(-)}(r_1)}{Q_K} 4\left(\frac{3}{4}\right)^{1/4} \mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}} \\
& \times \frac{1}{2}\left[\frac{1}{K-\mathrm{i}\sqrt{\frac{4}{3}E}}+\frac{1}{K+\mathrm{i}\sqrt{\frac{4}{3}E}}\right]\int\limits_0^{r_0} \mathrm{d}r_1'\, u_{Q_K}^{(-)*}(r_1')V(r_1') + O\left(\frac{1}{R_1^2}\right) \\
= & -\frac{4}{\pi}\left(\frac{3}{4}\right)^{1/4} \mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\int\limits_{K_0}^{\infty} \mathrm{d}K\, \frac{u_{Q_K}^{(-)}(r_1)}{Q_K}\frac{2K}{K^2+\frac{4}{3}E} \\
& \times \int\limits_0^{r_0} \mathrm{d}r_1'\, u_{Q_K}^{(-)*}(r_1')V(r_1') + O\left(\frac{1}{R_1^2}\right) \\
= & -\frac{4}{\pi}\left(\frac{3}{4}\right)^{1/4} \mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\int\limits_{K_0}^{\infty} \mathrm{d}K\, \frac{u_{Q_K}^{(-)}(r_1)}{Q_K}\frac{2K}{\frac{4}{3}Q_K^2} \\
& \times \int\limits_0^{r_0} \mathrm{d}r_1'\, u_{Q_K}^{(-)*}(r_1')V(r_1') + O\left(\frac{1}{R_1^2}\right),
\end{aligned} \tag{B.14}$$

where we have used the relation $E = Q_K^2 - \frac{3}{4}K^2$ in the last equality of Eq.(B.14). Performing the back transformation of the various quantities according to

$$E = Q_K^2 - \frac{3}{4}K^2 \longrightarrow E = k^2 + \frac{3}{4}Q_k^2 \tag{B.15}$$

and Eq. (B.7) yields the final form of $H_2(r_1,R_1)$,

$$\begin{aligned}
H_2(r_1,R_1) \backsimeq & -\frac{8}{\pi}\left(\frac{3}{4}\right)^{1/4} \mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\int\limits_{\sqrt{E}}^{\infty} \mathrm{d}k\, \frac{k}{K}\frac{4}{3}\frac{u_k^{(-)}(r_1)}{k}\frac{K}{\frac{4}{3}k^2} \\
& \times \int\limits_0^{r_0} \mathrm{d}r_1'\, u_k^{(-)*}(r_1')V(r_1') + O\left(\frac{1}{R_1^2}\right) \\
= & -\frac{8}{\pi}\left(\frac{3}{4}\right)^{1/4} \mathrm{A}\left(\arctan\frac{1}{\sqrt{3}}\right)\frac{\mathrm{e}^{\mathrm{i}\sqrt{\frac{4}{3}E}R_1}}{R_1^{3/2}}\int\limits_{\sqrt{E}}^{\infty} \mathrm{d}k\, u_k^{(-)}(r_1)\frac{1}{k^2} \\
& \times \int\limits_0^{r_0} \mathrm{d}r_1'\, u_k^{(-)*}(r_1')V(r_1') + O\left(\frac{1}{R_1^2}\right).
\end{aligned} \tag{B.16}$$

Because $K_0(R_1) \to 0$ for $R_1 \to \infty$ the lower integral boundary of the k-integral in Eq. (B.16) due to Eq. (B.15) becomes $\sqrt{E}$.

In the limit $r_1 \to \infty$ and R_1 fixed, the K-integration interval $\left[\sqrt{\frac{4}{3}E};\infty\right]$ was not considered in

Eq. (3.64) and yields the correction term

$$C(r_1, R_1) = -\frac{2}{\pi} \int\limits_{\sqrt{\frac{4}{3}E}}^{\infty} \mathrm{d}K \; \sin(KR_1) w_{q_K}(r_1) \int\limits_0^{r_1} \mathrm{d}r_1' \; \frac{u_{q_K}^{(+)}(r_1')}{q_K} \int\limits_0^{\infty} \mathrm{d}R_1' \; \sin(KR_1')V(r_1')Q(r_1', R_1') \,. \tag{B.17}$$

to the wave function $u(r_1, R_1)$ in Eq. (3.65). The wave number q_K is now considered to be imaginary because of $E = q_K^2 + \frac{3}{4}K^2$. We are not interested in calculating the integrals in Eq. (B.17), but we want to determine the leading behavior of $C(r_1, R_1)$ for large values of r_1, which results from $q_K \approx 0$. Then one has $\lim\limits_{q\to 0} \frac{u_q^{(+)}(r)}{q} = O(1)$ from [6] which allows us to estimate the correction term to be of the order $O\left(\frac{1}{r_1^2}\right)$ [6].

C Transformation of Eq. (3.72) into polar coordinates

The coordinates and momenta are transformed according to Eq. (3.74),

$$r_1 = \rho\cos\varphi \qquad q_K = \sqrt{E}\cos\alpha$$
$$R_1 = \sqrt{\frac{3}{4}}\rho\sin\varphi \qquad K = \sqrt{\frac{4}{3}E}\sin\alpha\,.$$

$$\begin{aligned}
u(r_1,R_1) &= -\frac{2}{\pi}\int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K\ \sin(KR_1)\mathrm{e}^{\mathrm{i}q_K r_1}\overline{T}(K)\\
&= -\frac{2}{\pi}\int_0^{\sqrt{\frac{4}{3}E}} \mathrm{d}K\ \frac{\mathrm{e}^{\mathrm{i}KR_1}-\mathrm{e}^{-\mathrm{i}KR_1}}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}q_K r_1}\overline{T}(K)\\
&= -\frac{2}{\pi}\int_0^{\pi/2} \mathrm{d}(\sin\alpha)\ \sqrt{\frac{4}{3}E}\frac{\left(\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\sin\alpha\sin\varphi}-\mathrm{e}^{-\mathrm{i}\rho\sqrt{E}\sin\alpha\sin\varphi}\right)}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos\alpha\cos\varphi}\overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&= -\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_0^{\pi/2} \mathrm{d}\alpha\ \frac{1}{2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}-\mathrm{e}^{-\mathrm{i}\rho\sqrt{E}\sin(\alpha+\varphi)}\right)\cos(\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&= -\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_0^{\pi/2} \mathrm{d}\alpha\ \frac{1}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}\cos(\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&\quad+\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_0^{-\pi/2} \mathrm{d}(-\alpha)\ \frac{1}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(-\alpha+\varphi)}\cos(-\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin(-\alpha)\right)\\
&= -\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_0^{\pi/2} \mathrm{d}\alpha\ \frac{1}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}\cos(\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&\quad-\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_0^{-\pi/2} \mathrm{d}\alpha\ \frac{1}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}\cos(\alpha)\ (-1)\cdot\overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&= -\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_0^{\pi/2} \mathrm{d}\alpha\ \frac{1}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}\cos(\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&\quad-\frac{2}{\pi}\sqrt{\frac{4}{3}E}\int_{-\pi/2}^{0} \mathrm{d}\alpha\ \frac{1}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}\cos(\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right)\\
&= -\frac{1}{\pi\mathrm{i}}\sqrt{\frac{4}{3}E}\int_{-\pi/2}^{\pi/2} \mathrm{d}\alpha\ \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\alpha-\varphi)}\cos(\alpha)\ \overline{T}\left(\sqrt{\frac{4}{3}E}\sin\alpha\right) = I_2\,.
\end{aligned} \tag{C.1}$$

In the sixth equality we used the fact that $\overline{T}(K)$ is an odd function of K.

D Transformation of Eq. (3.63) into polar coordinates

The transformation equations of the coordinates and momenta in Eq. (3.82) read

$$r_1 = \rho \sin\beta \qquad k = \sqrt{E}\sin\vartheta$$
$$R_1 = \sqrt{\frac{3}{4}}\rho\cos\beta \qquad Q_k = \sqrt{\frac{4}{3}E}\cos\vartheta\,.$$

For $u_k^{(-)}(r_1)$ we use its asymptotic form $u_k^{(-)}(r_1) \backsimeq \mathrm{e}^{-\mathrm{i}\delta(k)}\sin(kr+\delta(k))$, as we investigate the case where both coordinates r_1 and R_1 tend to infinity.

$$\begin{aligned}
I_1 &= -\frac{8}{3\pi}\int\limits_0^{\sqrt{E}} \mathrm{d}k\; u_k^{(-)}(r_1)\mathrm{e}^{\mathrm{i}Q_kR_1}T(k) = -\frac{8}{3\pi}\int\limits_0^{\sqrt{E}} \mathrm{d}k\; \mathrm{e}^{-\mathrm{i}\delta(k)}\frac{\mathrm{e}^{\mathrm{i}(kr_1+\delta(k))}-\mathrm{e}^{-\mathrm{i}(kr_1+\delta(k))}}{2\mathrm{i}}\mathrm{e}^{\mathrm{i}Q_kR_1}T(k)\\
&= -\frac{8}{3\pi}\frac{1}{2\mathrm{i}}\sqrt{E}\int\limits_0^{\pi/2}\mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{-\mathrm{i}\delta(\sqrt{E}\sin\vartheta)}\left(\mathrm{e}^{\mathrm{i}(\rho\sqrt{E}\sin\beta\sin\vartheta+\delta(\sqrt{E}\sin\vartheta))}-\mathrm{e}^{-\mathrm{i}(\rho\sqrt{E}\sin\beta\sin\vartheta+\delta(\sqrt{E}\sin\vartheta))}\right)\\
&\quad\times\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos\beta\cos\vartheta}T\left(\sqrt{E}\sin\vartheta\right)\\
&= -\frac{8}{3\pi}\frac{1}{2\mathrm{i}}\sqrt{E}\int\limits_0^{\pi/2}\mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\sin\beta\sin\vartheta}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos\beta\cos\vartheta}T\left(\sqrt{E}\sin\vartheta\right)\\
&\quad+\frac{8}{3\pi}\frac{1}{2\mathrm{i}}\sqrt{E}\int\limits_0^{\pi/2}\mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{-\mathrm{i}\delta(\sqrt{E}\sin\vartheta)}\mathrm{e}^{-\mathrm{i}(\rho\sqrt{E}\sin\beta\sin\vartheta+\delta(\sqrt{E}\sin\vartheta))}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos\beta\cos\vartheta}T\left(\sqrt{E}\sin\vartheta\right)
\end{aligned} \tag{D.1}$$

We now focus on the integral in the second term of the fourth equality of Eq. (D.1),

$$\begin{aligned}
&\int\limits_0^{-\pi/2}\mathrm{d}(-\vartheta)\;\cos(-\vartheta)\mathrm{e}^{-\mathrm{i}\delta(\sqrt{E}\sin(-\vartheta))}\mathrm{e}^{-\mathrm{i}\rho\sqrt{E}\sin\beta\sin(-\vartheta)}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos\beta\cos(-\vartheta)}\mathrm{e}^{-\mathrm{i}\delta(\sqrt{E}\sin(-\vartheta))}T\left(\sqrt{E}\sin(-\vartheta)\right)\\
&= -\int\limits_0^{-\pi/2}\mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{-\mathrm{i}\delta(-\sqrt{E}\sin\vartheta)}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}(\sin\beta\sin\vartheta+\cos\beta\cos\vartheta)}\underbrace{\mathrm{e}^{-\mathrm{i}\delta(-\sqrt{E}\sin\vartheta)}T\left(-\sqrt{E}\sin\vartheta\right)}_{\text{odd function of }k=\sqrt{E}\sin\vartheta}\\
&= -\int\limits_0^{-\pi/2}\mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{\mathrm{i}\delta(\sqrt{E}\sin\vartheta)}\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta)}(-1)\mathrm{e}^{-\mathrm{i}\delta(\sqrt{E}\sin\vartheta)}T\left(\sqrt{E}\sin\vartheta\right)\\
&= -\int\limits_{-\pi/2}^{0}\mathrm{d}\vartheta\;\cos\vartheta\,\mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta)}T\left(\sqrt{E}\sin\vartheta\right)\,.
\end{aligned} \tag{D.2}$$

We made use of the fact that $\delta(k)$ and $\mathrm{e}^{-\mathrm{i}\delta(k)}T(k)$ are odd functions of $k = \sqrt{E}\sin\vartheta$ and of the identity $\cos(x \pm y) = \cos x \cos y \mp \sin x \sin y$. Finally Eq.(D.1) reads

$$\begin{aligned} I_1 &= -\frac{4\sqrt{E}}{3\pi\mathrm{i}} \left[\int\limits_0^{\pi/2} \mathrm{d}\vartheta \ \cos\vartheta \, \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta)} T\left(\sqrt{E}\sin\vartheta\right) + \int\limits_{-\pi/2}^{0} \mathrm{d}\vartheta \ \cos\vartheta \, \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta)} T\left(\sqrt{E}\sin\vartheta\right) \right] \\ &= -\frac{4\sqrt{E}}{3\pi\mathrm{i}} \int\limits_{-\pi/2}^{\pi/2} \mathrm{d}\vartheta \ \cos\vartheta \, \mathrm{e}^{\mathrm{i}\rho\sqrt{E}\cos(\vartheta-\beta)} T\left(\sqrt{E}\sin\vartheta\right) . \end{aligned} \tag{D.3}$$

E Detailed treatment of Eq. (3.103)

In this section we consider the left hand side of Eq. (3.103),

$$\begin{aligned} &\iint_D \mathrm{d}r\,\mathrm{d}R\,\varphi_\mu(r,R)\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V(r)-\frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R^2}-E\right]u(r,R) \\ &= -\int_0^A \mathrm{d}R \int_0^a \mathrm{d}r\;\varphi_\mu(r,R)\frac{\mathrm{d}^2u}{\mathrm{d}r^2}-\frac{3}{4}\int_0^a \mathrm{d}r\int_0^A \mathrm{d}R\;\varphi_\mu(r,R)\frac{\mathrm{d}^2u}{\mathrm{d}R^2}+\varphi_\mu(r,R)[V(r)-E]u(r,R) \end{aligned} \tag{E.1}$$

and solve the occurring integrals. We can rewrite the terms containing second derivatives in Eq. (E.1) using the product rule twice (suppressing factors and the dependencies of the functions on spatial coordinates)

$$\frac{\mathrm{d}^2}{\mathrm{d}R^2}(\varphi_\mu u)=\frac{\mathrm{d}}{\mathrm{d}R}\left(\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}u+\varphi_\mu\frac{\mathrm{d}u}{\mathrm{d}R}\right)=\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2}u+\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\frac{\mathrm{d}u}{\mathrm{d}R}+\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\frac{\mathrm{d}u}{\mathrm{d}R}+\varphi_\mu\frac{\mathrm{d}^2u}{\mathrm{d}R^2} \tag{E.2}$$

and isolate the term which occurs in Eq. (E.1),

$$\varphi_\mu\frac{\mathrm{d}^2u}{\mathrm{d}R^2}=\frac{\mathrm{d}^2}{\mathrm{d}R^2}(\varphi_\mu u)-2\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\frac{\mathrm{d}u}{\mathrm{d}R}-\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2}u\,. \tag{E.3}$$

Using relation (E.3), the integrals in the second line of Eq. (E.1) can be calculated beginning with the second one,

$$
\begin{aligned}
&-\frac{3}{4}\int_0^A \mathrm{d}R\,\varphi_\mu(r,R)\frac{\mathrm{d}^2 u}{\mathrm{d}R^2} = -\frac{3}{4}\int_0^A \mathrm{d}R\,\left[\frac{\mathrm{d}^2}{\mathrm{d}R^2}\left[\varphi_\mu(r,R)u(r,R)\right] - 2\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\frac{\mathrm{d}u}{\mathrm{d}R} - \frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2}u\right] \\
&= -\frac{3}{4}\,\frac{\mathrm{d}}{\mathrm{d}R}(\varphi_\mu(r,R)u(r,R))\bigg|_0^A + \frac{3}{2}\int_0^A \mathrm{d}R\,\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\frac{\mathrm{d}u}{\mathrm{d}R} + \frac{3}{4}\int_0^A \mathrm{d}R\,u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2} \\
&= -\frac{3}{4}\left(u(r,R)\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R} + \varphi_\mu(r,R)\frac{\mathrm{d}u}{\mathrm{d}R}\right)\bigg|_0^A + \frac{3}{2}\left[\varphi_\mu(r,R)\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_0^A - \int_0^A \mathrm{d}R\,\varphi_\mu(r,R)\frac{\mathrm{d}^2 u}{\mathrm{d}R^2}\right] \\
&\quad + \frac{3}{4}\int_0^A \mathrm{d}R\,u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2} \qquad \text{(E.4)} \\
&= -\frac{3}{4}\left[u(r,A)\,\underbrace{\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\bigg|_{R=A}}_{=0} - \underbrace{u(r,0)}_{=0}\,\frac{\mathrm{d}\varphi_\mu}{\mathrm{d}R}\bigg|_{R=0} + \varphi_\mu(r,A)\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} - \underbrace{\varphi_\mu(r,0)}_{=0}\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=0}\right] \\
&\quad + \frac{3}{2}\varphi_\mu(r,A)\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} - \frac{3}{2}\underbrace{\varphi_\mu(r,0)}_{=0}\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=0} - \frac{3}{2}\int_0^A \mathrm{d}R\,\varphi_\mu(r,R)\frac{\mathrm{d}^2 u}{\mathrm{d}R^2} + \frac{3}{4}\int_0^A \mathrm{d}R\,u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2} \\
&= \frac{3}{4}\varphi_\mu(r,A)\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} - \frac{3}{2}\int_0^A \mathrm{d}R\,\varphi_\mu(r,R)\frac{\mathrm{d}^2 u}{\mathrm{d}R^2} + \frac{3}{4}\int_0^A \mathrm{d}R\,u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2}\,.
\end{aligned}
$$

We integrated by parts in the second line of Eq. (E.4) and in the fifth and sixth line we made use of the boundary conditions (3.95),

$$
\varphi_\mu(0,R) = \varphi_\mu(r,0) = \frac{\partial\varphi_\mu(r,R)}{\partial r}\bigg|_{r=a} = \frac{\partial\varphi_\mu(r,R)}{\partial R}\bigg|_{R=A} = 0\,.
$$

Additionally, $u(r,0) = 0$ since we integrate over the domain D and inside D we have

$$
u(r,0) = \sum_\mu c_\mu\varphi_\mu(r,0) = 0\,. \qquad \text{(E.5)}
$$

Finally we get the result

$$
\frac{3}{4}\int_0^A \mathrm{d}R\,\varphi_\mu(r,R)\frac{\mathrm{d}^2 u}{\mathrm{d}R^2} = \frac{3}{4}\varphi_\mu(r,A)\,\frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} + \frac{3}{4}\int_0^A \mathrm{d}R\,u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2} \qquad \text{(E.6)}
$$

and analogously

$$\int_0^a \mathrm{d}r\ \varphi_\mu(r,R)\frac{\mathrm{d}^2u}{\mathrm{d}r^2} = \varphi_\mu(a,R)\ \frac{\mathrm{d}u}{\mathrm{d}r}\bigg|_{r=a} + \int_0^a \mathrm{d}r\ u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}r^2}\,. \tag{E.7}$$

Inserting them into Eq. (E.1) yields

$$\begin{aligned}
&-\int_0^A \mathrm{d}R\ \varphi_\mu(a,R)\ \frac{\mathrm{d}u}{\mathrm{d}r}\bigg|_{r=a} - \int_0^A \mathrm{d}R\ \int_0^a \mathrm{d}r\ u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}r^2} \\
&\quad -\frac{3}{4}\int_0^a \mathrm{d}r\ \varphi_\mu(r,A)\ \frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} - \frac{3}{4}\int_0^a \mathrm{d}r\ \int_0^A \mathrm{d}R\ u(r,R)\frac{\mathrm{d}^2\varphi_\mu}{\mathrm{d}R^2} + \varphi_\mu(r,R)[V(r)-E]u(r,R) \\
&= -\int_0^A \mathrm{d}R\ \varphi_\mu(a,R)\ \frac{\mathrm{d}u}{\mathrm{d}r}\bigg|_{r=a} - \frac{3}{4}\int_0^a \mathrm{d}r\ \varphi_\mu(r,A)\ \frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} \\
&\quad + \int_0^A \mathrm{d}R\int_0^a \mathrm{d}r\ u(r,R)\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R^2} - E\right]\varphi_\mu(r,R) \\
&= -\int_0^A \mathrm{d}R\ \varphi_\mu(a,R)\ \frac{\mathrm{d}u}{\mathrm{d}r}\bigg|_{r=a} - \frac{3}{4}\int_0^a \mathrm{d}r\ \varphi_\mu(r,A)\ \frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} \\
&\quad + \int_0^A \mathrm{d}R\int_0^a \mathrm{d}r\ (E_\mu - E)u(r,R)\varphi_\mu(r,R) \\
&= -\int_0^A \mathrm{d}R\ \varphi_\mu(a,R)\ \frac{\mathrm{d}u}{\mathrm{d}r}\bigg|_{r=a} - \frac{3}{4}\int_0^a \mathrm{d}r\ \varphi_\mu(r,A)\ \frac{\mathrm{d}u}{\mathrm{d}R}\bigg|_{R=A} + (E_\mu - E)c_\mu
\end{aligned} \tag{E.8}$$

In the third equality we applied Eq. (3.94),

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) - \frac{3}{4}\frac{\mathrm{d}^2}{\mathrm{d}R^2} - E_\mu\right]\varphi_\mu(r,R) = 0$$

and in the last line we used the definition of the expansion coefficients (3.101) for the interior wave function,

$$c_\mu = \iint_D \mathrm{d}r\,\mathrm{d}R\ \varphi_\mu(r,R)u(r,R)\,.$$

F Calculation of the terms $H_i^{(1)}(R_i)$ and $H_i^{(2)}(r_i, R_i)$ in Eqs. (4.31) and (4.32)

We start with the integral neglecting constant factors

$$I = 2\mu_{i(jk)} \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \, \frac{\sin[Q(R_i - R_i')]}{Q} \sum_{\substack{j=1 \\ j \neq i}}^{3} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\,\frac{m_i}{m_i+m_k}\,R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \tag{F.1}$$

and define

$$I_j = 2\mu_{i(jk)} \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \, \frac{\sin[Q(R_i - R_i')]}{Q} \, \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\,\frac{m_i}{m_i+m_k}\,R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \, . \tag{F.2}$$

In analogy to Appendix B we integrate by parts two times, yielding

$$
\begin{aligned}
I_j =& \frac{2\mu_{i(jk)}}{Q} \left[\frac{1}{Q} \cos[Q(R_i - R_i')] \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \right]\Bigg|_{R_i}^{\infty} \\
&- \frac{2\mu_{i(jk)}}{Q^2} \int_{R_i}^{\infty} \mathrm{d}R_i' \ \cos[Q(R_i - R_i')] \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*} \left(\mathrm{i}\sqrt{2\mu_{j(ik)}E}R_i' \frac{m_i}{m_i+m_k}/\sin\varphi_j^* - \frac{3}{2} \right)}{R_i'^{5/2}} \\
\backsimeq& \frac{2\mu_{i(jk)}}{Q^2} \left[0 - \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} \right] \\
&- \frac{2\mu_{i(jk)}}{Q^2} \int_{R_i}^{\infty} \mathrm{d}R_i' \ \cos[Q(R_i - R_i')] \frac{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}/\sin\varphi_j^* \cdot \mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \\
=& - \frac{2\mu_{i(jk)}}{Q^2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
&- \frac{2\mu_{i(jk)}}{Q^2} \left[-\frac{1}{Q} \sin[Q(R_i - R_i')] \frac{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}/\sin\varphi_j^* \cdot \mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \right]\Bigg|_{R_i}^{\infty} \\
&- \frac{2\mu_{i(jk)}}{Q^2} \int_{R_i}^{\infty} \mathrm{d}R_i' \ \frac{\sin[Q(R_i - R_i')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \left(-\frac{m_i}{m_i+m_k}\mu_{j(ik)}E/\sin^2\varphi_j^* \right) \\
=& - \frac{2\mu_{i(jk)}}{Q^2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} - \frac{2\mu_{j(ik)}}{Q^2}[0 - 0] \\
&+ \frac{2\mu_{i(jk)}}{Q^2} \int_{R_i}^{\infty} \mathrm{d}R_i' \ \frac{\sin[Q(R_i - R_i')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \frac{m_i}{m_i+m_k}\mu_{j(ik)}E/\sin^2\varphi_j^* \\
=& - \frac{2\mu_{i(jk)}}{Q^2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
&+ \frac{1}{Q^2} \left[2\mu_{i(jk)} \int_{R_i}^{\infty} \mathrm{d}R_i' \ \frac{\sin[Q(R_i - R_i')]}{Q} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i'/\sin\varphi_j^*}}{R_i'^{3/2}} \right] \frac{m_i}{m_i+m_k}\mu_{j(ik)}E/\sin^2\varphi_j^* \, .
\end{aligned}
\tag{F.3}
$$

Again, the term proportional to $R_i^{'-5/2}$ in the second line of Eq. (F.3) was neglected in the following equalities. From Eq. (F.3) we can calculate the integral I_j,

$$\begin{aligned}
I_j - \frac{1}{Q^2} I_2 \frac{m_i}{m_i+m_k} \mu_{j(ik)} E / \sin^2\varphi_j^* &= -\frac{2\mu_{i(jk)}}{Q^2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
I_j\left(1 - \frac{1}{Q^2}\frac{m_i}{m_i+m_k}\mu_{j(ik)}E/\sin^2\varphi_j^*\right) &= -\frac{2\mu_{i(jk)}}{Q^2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
I_j\left(E - \frac{Q^2(m_i+m_k)\sin^2\varphi_j^*}{m_i\mu_{j(ik)}}\right) &= \frac{2\mu_{i(jk)}}{\mu_{j(ik)}}\frac{m_i+m_k}{m_i}\sin^2\varphi_j^* \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
I_j &= \frac{2\mu_{i(jk)}(m_i+m_k)\sin^2\varphi_j^*}{m_i\mu_{j(ik)}\left(E - \frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i^{3/2}}\,.
\end{aligned} \tag{F.4}$$

Consequently,

$$I = \sum_{\substack{j=1\\ j\neq i}}^{3} I_j = \sum_{\substack{j=1\\ j\neq i}}^{3} \frac{2\mu_{i(jk)}(m_i+m_k)\sin^2\varphi_j^*}{m_i\mu_{j(ik)}\left(E - \frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i^{3/2}}\,. \tag{F.5}$$

The total expression for the first additional term of the asymptotic form of $u_i(r_i,R_i)$ in the limit $R_i\to\infty$ and r_i fixed, reads

$$\begin{aligned}
H_i^{(1)}(R_i) = &\sum_{\substack{j=1\\ j\neq i}}^{3} (2\mu_{j(ik)})^{-1/4}\left(\frac{m_i+m_k}{m_i}\sin\varphi_j^*\right)^{5/2} \mathrm{A}(\varphi_j^*)\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i/\sin\varphi_j^*}}{R_i^{3/2}} \\
&\times \frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E - \frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)} \int_0^{r_{0i}} \mathrm{d}r_i'\; r_i' u_i^b(r_i') V_i(r_i')\,.
\end{aligned} \tag{F.6}$$

The second term $H_i^{(2)}(r_i,R_i)$ (Eq. (4.32)) is obtained by integrating over the k-interval $\left[\sqrt{2\mu_{i(jk)}E};\infty\right]$, where the wavenumber Q_k due to $E=\frac{1}{2\mu_{jk}}k^2+\frac{1}{2\mu_{i(jk)}}Q_k^2$ becomes a complex quantity,

$$Q_k \hat{=} \mathrm{i}K \qquad \text{and} \qquad k \hat{=} Q_K\,, \tag{F.7}$$

while K and Q_K are real quantities. Then,

$$E = \frac{1}{2\mu_{jk}}k^2 + \frac{1}{2\mu_{i(jk)}}Q_k^2 \longrightarrow E = \frac{1}{2\mu_{jk}}Q_K^2 - \frac{1}{2\mu_{i(jk)}}K^2\,. \tag{F.8}$$

Differentiating the second relation in Eq. (F.8) leads to

$$\begin{aligned} \frac{1}{2\mu_{jk}} 2k\mathrm{d}k &= \frac{1}{2\mu_{i(jk)}} 2K\mathrm{d}K \\ \mathrm{d}k &= \frac{\mu_{jk}}{\mu_{i(jk)}} \frac{K}{k} \mathrm{d}K \,, \end{aligned} \tag{F.9}$$

where we used $k \hat{=} Q_K$. So we can transform the integrals over k, resulting when inserting the Green's function (4.29a) into Eq. (4.11),

$$\begin{aligned} &- \cdot \frac{4\mu_{i(jk)}}{\pi} \int\limits_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \; u_k^{(-)}(r_i) \mathrm{e}^{\mathrm{i}Q_k R_i} \int\limits_0^{R_i} \mathrm{d}R_i' \; \frac{\sin(Q_k R_i')}{Q_k} \int\limits_0^{\infty} \mathrm{d}r_i' \; u_k^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \\ &- \cdot \frac{4\mu_{i(jk)}}{\pi} \int\limits_0^{\sqrt{2\mu_{jk}E}} \mathrm{d}k \; u_k^{(-)}(r_i) \frac{\sin(Q_k R_i')}{Q_k} \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \; \mathrm{e}^{\mathrm{i}Q_k R_i} \int\limits_0^{\infty} \mathrm{d}r_i' \; u_k^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \,, \end{aligned} \tag{F.10}$$

into integrals over K

$$\begin{aligned} H_i^{(2)}(r_i, R_i) =& - \frac{4\mu_{i(jk)}}{\pi} \int\limits_0^{\infty} \mathrm{d}K \; \frac{\mu_{jk}}{\mu_{i(jk)}} \frac{K}{k} \cdot \frac{u_{Q_K}^{(-)}(r_i)}{\mathrm{i}K} \\ & \times \left[\mathrm{e}^{\mathrm{i}^2 K R_i} \int\limits_0^{R_i} \mathrm{d}R_i' \sin(\mathrm{i}KR_i') + \sin(\mathrm{i}KR_i) \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \mathrm{e}^{\mathrm{i}^2 K R_i'} \right] \int\limits_0^{r_0} \mathrm{d}r_i' u_{Q_K}^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \\ =& - \frac{4}{\pi} \int\limits_0^{\infty} \mathrm{d}K \; \mu_{jk} \frac{u_{Q_K}^{(-)}(r_i)}{\mathrm{i}k} \left[\mathrm{e}^{-KR_i} \int\limits_0^{R_i} \mathrm{d}R_i' \; \mathrm{i} \cdot \sinh(KR_i') + \mathrm{i} \cdot \sinh(KR_i) \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \; \mathrm{e}^{-KR_i'} \right] \\ & \times \int\limits_0^{r_0} \mathrm{d}r_i' \; u_{Q_K}^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \\ =& - \frac{4}{\pi} \int\limits_0^{\infty} \mathrm{d}K \; \mu_{jk} \frac{u_{Q_K}^{(-)}(r_i)}{Q_K} \left[\mathrm{e}^{-KR_i} \int\limits_0^{R_i} \mathrm{d}R_i' \; \sinh(KR_i') + \sinh(KR_i) \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \; \mathrm{e}^{-KR_i'} \right] \\ & \times \int\limits_0^{r_0} \mathrm{d}r_i' \; u_{Q_K}^{(-)*}(r_i') V_i(r_i') Q_i(r_i', R_i') \,. \end{aligned} \tag{F.11}$$

The integration over K is split according to $\int_0^{\infty} \mathrm{d}K = \int_0^{K_0(R_i)} \mathrm{d}K + \int_{K_0(R_i)}^{\infty} \mathrm{d}K$ with $K_0(R_i) \cdot R_i \to \infty$ and $K_0(R_i) \to 0$ for $R_i \to \infty$. For $K \geq K_0$ we solve the integral over R_i' via integration by parts and use the asymptotic form of $Q_i(r_i, R_i)$ from Eq. (4.28) (considering R_i-dependent terms only),

$$
\begin{aligned}
\tilde{H}_{ij}^{(1)}(r_i, R_i) &= \sinh(KR_i) \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \, \mathrm{e}^{-KR_i'} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*}}{R_i'^{3/2}} \\
&= \sinh(KR_i) \int\limits_{R_i}^{\infty} \mathrm{d}R_i' \, \mathrm{e}^{-KR_i'} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*}}{R_i'^{3/2}} \\
&= \frac{\sinh(KR_i)}{\mathrm{i}\sqrt{2\mu_{j(ik)}E\frac{m_i}{m_i+m_k}} / \sin\varphi_j^* - K} \cdot \left. \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*} - KR_i'}{R_i'^{3/2}} \right|_{R_i}^{\infty} + O\left(\frac{1}{R_i^{5/2}}\right) \\
&\backsimeq 0 - \frac{1}{2}\left(\mathrm{e}^{KR_i} - \mathrm{e}^{-KR_i}\right) \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i / \sin\varphi_j^* - KR_i}}{R_i^{3/2}\left(\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^* - K\right)} \\
&= \frac{1}{2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i / \sin\varphi_j^*}}{R_i^{3/2}\left(K - \mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} / \sin\varphi_j^*\right)} + O\left(\mathrm{e}^{-2K_0R_i}\right) .
\end{aligned}
\tag{F.12}
$$

Finally $\tilde{H}_i^{(1)}(r_i, R_i)$, which is the sum over $\tilde{H}_{ij}^{(1)}(r_i, R_i)$ with all parts of asymptotic $Q_i(r_i, R_i)$, reads

$$
\tilde{H}_i^{(1)}(r_i, R_i) = \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{3} (2\mu_{j(ik)})^{-1/4} \left(\frac{m_i + m_k}{m_i}\right)^{3/2} \left(\sin\varphi_j^*\right)^{5/2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i / \sin\varphi_j^*}}{R_i^{3/2}\left(K - \mathrm{i}\sqrt{2\mu_{j(ik)}E\frac{m_i}{m_i+m_k}} / \sin\varphi_j^*\right)} .
\tag{F.13}
$$

The remaining term (including the R_i-dependent part of asymptotic $Q_i(r_i, R_i)$ only) is calculated as

$$
\begin{aligned}
\tilde{H}_{ij}^{(2)}(r_i, R_i) =& \mathrm{e}^{-KR_i} \int\limits_{0}^{R_i} \mathrm{d}R_i' \frac{\mathrm{e}^{KR_i'} - \mathrm{e}^{-KR_i'}}{2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*}}{R_i'^{3/2}} \\
=& \frac{1}{2} \frac{\mathrm{e}^{-KR_i}}{K + \mathrm{i}\sqrt{2\mu_{j(ik)}E\frac{m_i}{m_i+m_k}} / \sin\varphi_j^*} \\
& \times \left[\left. \frac{\mathrm{e}^{KR_i' + \mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*} - \mathrm{e}^{-KR_i' + \mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*}}{R_i'^{3/2}} \right] \right|_{0}^{R_i} + O\left(\frac{1}{R_i^{5/2}}\right) \\
\backsimeq& \frac{1}{2} \frac{\mathrm{e}^{-KR_i}}{K + \mathrm{i}\sqrt{2\mu_{j(ik)}E\frac{m_i}{m_i+m_k}} / \sin\varphi_j^*} \left. \frac{\mathrm{e}^{KR_i' + \mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i' / \sin\varphi_j^*}}{R_i'^{3/2}} \right|_{0}^{R_i} + O\left(\mathrm{e}^{-2K_0R_i}\right) \\
\backsimeq& \frac{1}{2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i / \sin\varphi_j^*}}{R_i^{3/2}\left(K + \mathrm{i}\sqrt{2\mu_{j(ik)}E\frac{m_i}{m_i+m_k}} / \sin\varphi_j^*\right)} .
\end{aligned}
\tag{F.14}
$$

Again, $\tilde{H}_i^{(2)}(r_i, R_i)$ is the sum over $\tilde{H}_{ij}^{(2)}(r_i, R_i)$ and contains the total asymptotic form of $Q_i(r_i, R_i)$,

$$\tilde{H}_i^{(2)}(r_i, R_i) = \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{3} (2\mu_{j(ik)})^{-1/4} \left(\frac{m_i + m_k}{m_i} \right)^{3/2} \left(\sin \varphi_j^* \right)^{5/2} \frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} R_i / \sin \varphi_j^*}}{R_i^{3/2} \left(K + \mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k} / \sin \varphi_j^* \right)} \tag{F.15}$$

Terms of order $R_i^{-\alpha}$ with $\alpha > \frac{3}{2}$ are neglected in Eqs. (F.12) and (F.14). In Eq. (F.14) we put $\int_0^{R_i} \mathrm{d}R_i' = \int_0^{d} \mathrm{d}R_i' + \int_d^{R_i} \mathrm{d}R_i'$, where d is such that the asymptotic form of $Q_i(r_i, R_i)$ can be applied and the lower boundary does not contribute. In the interval $0 \leq K \leq K_0$ again we can estimate the correction term to be of the order $O\left(\frac{1}{R_i^2}\right)$ for $R_i \to \infty$. The the total term $H_i^{(2)}(r_i, R_i)$ is obtained by inserting $\tilde{H}_i^{(1)}$ and $\tilde{H}_i^{(2)}$ into Eq. (F.11) and adding the estimated correction term of order $O\left(\frac{1}{R_i^2}\right)$, yielding

$$
\begin{aligned}
H_i^{(2)}(r_i,R_i) =& -\frac{4}{\pi}\int\limits_{K_0}^{\infty}\mathrm{d}K\;\mu_{jk}\frac{u_{Q_K}^{(-)}(r_i)}{Q_K}\tilde{H}_i^{(1)}(r_i,R_i)+\tilde{H}_i^{(2)}(r_i,R_i)\int\limits_{0}^{r_0}\mathrm{d}r_i'\;u_{Q_K}^{(-)*}(r_i')V(r_i')+O\left(\frac{1}{R_i^2}\right)\\
\backsimeq& -\frac{4}{\pi}\int\limits_{K_0}^{\infty}\mathrm{d}K\;\mu_{jk}\frac{u_{Q_K}^{(-)}(r_i)}{Q_K}\frac{1}{2}\sum_{\substack{j=1\\ j\neq i}}^{3}\left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\\
&\times\left[\frac{1}{K-\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}/\sin\varphi_j^*}+\frac{1}{K+\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}/\sin\varphi_j^*}\right]\\
&\times\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}}\int\limits_{0}^{r_0}\mathrm{d}r_i'\;u_{Q_K}^{(-)*}(r_i')V(r_i')+O\left(\frac{1}{R_i^2}\right)\\
=& -\frac{2}{\pi}\sum_{\substack{j=1\\ j\neq i}}^{3}\left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}}\\
&\times\int\limits_{K_0}^{\infty}\mathrm{d}K\;\mu_{jk}\frac{u_{Q_K}^{(-)}(r_i)}{Q_K}\frac{2K}{K^2+2\mu_{j(ik)}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\int\limits_{0}^{r_0}\mathrm{d}r_i'\;u_{Q_K}^{(-)*}(r_i')V(r_i')+O\left(\frac{1}{R_i^2}\right)\\
=& -\frac{2}{\pi}\sum_{\substack{j=1\\ j\neq i}}^{3}\left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}}\\
&\times\int\limits_{K_0}^{\infty}\mathrm{d}K\;\mu_{jk}\frac{u_{Q_K}^{(-)}(r_i)}{Q_K}\frac{2K}{\frac{\mu_{i(jk)}}{\mu_{jk}}Q_K^2-2\mu_{i(jk)}E+2\mu_{j(ik)}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\\
&\times\int\limits_{0}^{r_0}\mathrm{d}r_i'\;u_{Q_K}^{(-)*}(r_i')V(r_i')+O\left(\frac{1}{R_i^2}\right)\\
=& -\frac{2}{\pi}\sum_{\substack{j=1\\ j\neq i}}^{3}\left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}}\\
&\times\int\limits_{\sqrt{2\mu_{jk}E}}^{\infty}\mathrm{d}k\;\frac{\mu_{i(jk)}}{\mu_{jk}}\frac{k}{K}\mu_{jk}\frac{u_k^{(-)}(r_i)}{k}\frac{2K}{\frac{\mu_{i(jk)}}{\mu_{jk}}k^2-2\mu_{i(jk)}E+2\mu_{j(ik)}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\\
&\times\int\limits_{0}^{r_0}\mathrm{d}r_i'\;u_k^{(-)*}(r_i')V(r_i')+O\left(\frac{1}{R_i^2}\right).
\end{aligned}
\tag{F.16}
$$

$$
\begin{aligned}
H_i^{(2)}(r_i,R_i) = &-\frac{4}{\pi}\sum_{\substack{j=1\\ j\neq i}}^{3}\left(2\mu_{j(ik)}\right)^{-1/4}\left(\frac{m_i+m_k}{m_i}\right)^{3/2}\sqrt{\sin\varphi_j^*}\;\mathrm{A}(\varphi_j^*)\frac{\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}R_i/\sin\varphi_j^*}}{R_i^{3/2}}\\
&\times\int\limits_{\sqrt{2\mu_{jk}E}}^{\infty}\mathrm{d}k\; u_k^{(-)}(r_i)\frac{1}{\frac{1}{\mu_{jk}}k^2-2E+2\frac{\mu_{j(ik)}}{\mu_{i(jk)}}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\int\limits_0^{r_0}\mathrm{d}r_i'\;u_k^{(-)*}(r_i')V(r_i')\\
&+O\left(\frac{1}{R_i^2}\right)\,.
\end{aligned}
\tag{F.17}
$$

We made use of the relation $E=\frac{1}{2\mu_{jk}}Q_K^2-\frac{1}{2\mu_{i(jk)}}K^2 \Rightarrow K^2=\frac{\mu_{i(jk)}}{\mu_{jk}}Q_K^2-2\mu_{i(jk)}E$ in the fourth equality of Eq.(F.16) and performed the back transformation according to

$$
E=\frac{1}{2\mu_{jk}}Q_K^2-\frac{1}{2\mu_{i(jk)}}K^2\longrightarrow E=\frac{1}{2\mu_{jk}}k^2+\frac{1}{2\mu_{i(jk)}}Q_k^2 \tag{F.18}
$$

by using Eqs. (F.7) and (F.9) in the fifth equality of Eq.(F.16). Because $K_0(R_i)\rightarrow 0$ for $R_i\rightarrow\infty$ the lower integral boundary of the k-integral in Eq. (F.16) due to Eq. (F.18) becomes $\sqrt{2\mu_{jk}E}$.

References

[1] E.P. Wigner, L. Eisenbud, Phys. Rev. **72**, 29 (1947)

[2] A.M. Lane, R.G. Thomas, Rev. Mod. Phys. **72**, 257-353 (1958)

[3] A.M. Lane, R.G. Thomas, Rev. Mod. Phys. **72**, 334-336 (1958)

[4] J.D. Jackson, Can. J. Phys. **34**, 767 (1956)

[5] W. Glöckle, Nucl. Phys. **271**, 620 (1970)

[6] W. Glöckle, Z. Physik **271**, 31-37 (1974)

[7] L.D. Faddeev, Soviet Phys. JETP **12**, 1014 (1961)

[8] E.W. Schmid, H. Ziegelmann, "The Quantum Mechanical Three-Body Problem", Vieweg, **ISBN** 3 528 0**8337** 9

[9] W. Glöckle, "The Quantum Mechanical Few-Body Problem", Springer Verlag, **ISBN**-13:978-3-642-82083-0

[10] R. Newton, "Scattering Theory of Waves and Particles", Second Edition, Springer Verlag, **ISBN** 0-387-**10950**-1

[11] N.G. De Bruijn "Asymptotic methods in Analysis", Dover Publications, Inc., New York **ISBN** 0-486-64221-6

[12] http://bolvan.ph.utexas.edu/ vadim/Classes/2011f/saddle.pdf, viewed on July 15, 2017

[13] P. Descouvemont, D. Baye, Reports on Progress in Physics **73**, 036301 (2010)

Acknowledgments

First I want to express gratitude to my supervisor Prof. Helmut Leeb. He spared no time and efforts to guide me through this thesis with great competence and experience. In many discussion we reviewed my ideas and I got new impulses and inspirations to proceed. It was often quite challenging since three-body reactions in the resonance regime have been treated only approximatively in literature up to now. Therefore I am glad that I got the chance to contribute to a new topic in nuclear physics.

Thanks to my colleague Thomas Srdinko for his helpfulness and advices in various matters related to my work.

I am grateful to have met colleagues and friends during my studies coming from different countries of the world who expanded my horizons not only in scientific fields.

Finally I want particularly thank my parents Maria and Franz and my brother Lukas for their great help and support in every sense during my studies.