Developments regarding three-body reaction channels within the R-matrix formalism

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Abstract. At low incident energies of nucleon-induced reaction cross sections exhibit a striking resonance structure which cannot properly be described by (semi-)microscopic models. Usually R-matrix theory is applied which provides a sufficiently accurate but phenomenological description of the resonance region. However, standard R-matrix theory is only suited for two-particle channels. Three- and many-particle channels which may occur at rather low incident energies and are usually treated in approximative or effective way. In this contribution an extension to unequal masses of the R-matrix formulation of Glöckle based on the Faddeev equation is performed and proper expressions for numerical implementation are given.

1 Introduction

A good knowledge of nuclear reaction cross sections is an important prerequisite not only for the design of nuclear devices and the development of novel nuclear technologies, but also for several applications e.g. materials science, nuclear medicine, geology and space research. Hence there exists a worldwide effort to establish nuclear data libraries which represent our best knowledge of reaction cross sections. This endeavour was started in the middle of the last century and was primarily focussed on neutron-induced reaction data. At present there exist several evaluated nuclear data libraries which represent our best quantitative knowledge of nuclear reaction data for a wide range of nuclei and projectiles. Especially, for neutron-induced reaction cross section of medium and heavy nuclei the libraries provide excellent description of cross sections up to neutron energies of 200 MeV.

At low incident energies the reaction cross sections exhibit striking resonance structures associated with many-nucleon effects. These phenomena cannot be properly reproduced by (semi-)microscopic nuclear models. Usually R-matrix theory \cite{1} is applied to obtain a sufficiently accurate but phenomenological description of the resonance region. However, the concept of standard R-matrix theory is only based on two-particle reaction channels. Thus three- and many-particle channels cannot be describe by standard R-matrix theory and are usually treated in an approximative way \cite{2}, e.g. by sequential processes. A similar difficulty arises also for capture channel, e.g. (n,γ) for which perturbative approaches are frequently applied.

In 1974 Glöckle \cite{3} proposed an R-matrix formulation based on Faddeev equations for reactions with three particles of equal mass in the exit channel. The availability of such an R-matrix treatment of three-particle channels would be of great interest, especially for light nuclear systems in which breakup channels may open in the resonance region. Albeit this three-particle R-matrix formalism is known for more than four decades we are not aware of any further development or application of the method.

In this contribution we focus on the extension of this formalism to channels with three particles of unequal mass in s-wave states. After this introduction we briefly revisit in Sect. 2 the concept and basic formulae of standard R-matrix theory. Especially, we discuss the difficulties arising in the treatment of three- and more-particle channels. The methods for three-particle channels are the focus of Sect. 3. After a short consideration of the sequential approach, introduced by Lane and Thomas \cite{2}, a more detailed sketch of the Faddeev based R-matrix formulation is given together with reformulated expressions suited for numerical implementation. Finally a summary and concluding remarks are given in Sect. 4.

2 The R-matrix formalism

2.1 Concept of R-matrix theory

Standard R-matrix theory is formulated for reactions of particle systems for which non-relativistic quantum mechanics is applicable. Hence creation and destruction processes of particles are excluded. Furthermore one assumes that only channels with two objects (e.g. nucleons or nuclei) are important. Hence channels with three or more objects are absent or negligible. In addition it is assumed that there exists in each channel a finite distance beyond that no mutual polarization of the objects occur. Consequently there exists a so-called channel surface which divides the space into an internal and an external region (Fig. 1). In the external region all quantities (potential, wave functions etc.) are given in terms of the distance \( r \) between the two particles.

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objects of the channel. The internal region is governed by the microscopic potential and leads to intriguing dependencies of the total wave function. In R-matrix theory the lack of detailed knowledge of the wave function in the internal region is effectively described by an expansion of a set of basis states in $r$ which is matched at the channel surface to the external region. A comprehensive and detailed description of the R-matrix formalism is given by Lane and Thomas [2]. In the following we give a brief sketch of basic relations of R-matrix theory which are relevant for the further developments described later. Here we follow Ref. [4] which provides an excellent and didactic introduction.

We start with a simple single-channel problem governed by a central potential $V(r)$ and described by the radial Schrödinger equation

$$ (T_r + V(r) - E) u_r(r) = 0 $$

with the kinetic energy operator

$$ T_r = -\frac{\hbar^2}{2\mu} \left( \frac{d^2}{dr^2} - \frac{\ell(\ell + 1)}{r^2} \right). $$

Here, $E$ is the energy, $\ell$ the orbital momentum quantum number and $\mu$ is the reduced mass of the channel. The potential is usually composed of a Coulomb part of infinite range and a short-ranged nuclear part. Introducing a matching radius $a$ sufficiently large that the nuclear part is negligible defines a proper channel surface and thus the separation of the space into an internal and an external region.

In the internal region the form of the radial wave function $u_r(r)$ is given in terms of the S-matrix element $U_l(E)$, i.e.

$$ u_r^{\text{int}}(r) = C_r [I_r(kr) - U_l \cdot O_l(kr)] \quad \text{for} \quad r \geq a , $$

where $k = \sqrt{2\mu E}/\hbar$. The incoming and outgoing functions $I_l = G_l - iF_l$ and $O_l = G_l + iF_l$ are defined in terms of the regular and irregular Coulomb functions $F_l$ and $G_l$, respectively.

In the internal region the radial wave function $u_r(r)$ is represented by an expansion over a finite set of $N$ linearly independent basis functions, $\varphi_j(r)$, $j = 1, \cdots, N$,

$$ u_r^{\text{int}}(r) = \sum_{j=1}^N c_j \varphi_j(r). \quad (4) $$

In order to describe a physical solution the basis functions $\varphi_j$ must vanish at $r = 0$, but they must not satisfy specific boundary conditions at the matching radius $r = a$.

As a solution of Eq. (1) the radial wave function $u_r(r)$ and its derivative $u'_r(r)$ must be continuous at each $r$-value in the domain $r \in [0, \infty]$ and especially at the matching radius $a$. The matching of the external wave function $u_e^{\text{ext}}$, Eq. (3) and the internal wave function $u_r^{\text{int}}$, Eq. (4), at the channel surface provides a boundary condition, which is conveniently expressed by the definition of the R-matrix $R_l(E)$,

$$ u_r(r = a) = R_l(E) \left[ au'_r(r = a) - Bu_r(r = a) \right] , \quad (5) $$

where $B$ is a dimensionless boundary parameter. The inverse of the R-matrix is directly related to the logarithmic derivative at the matching radius.

The R-matrix takes a particularly convenient form for a Hamiltonian which is hermitean on the domain of the internal region $r \in [0, a]$. This is not satisfied for the Hamiltonian of Eq. (1), but can easily be restored by introducing the Bloch operator [5],

$$ \tilde{L} = \frac{\hbar^2}{2\mu} \delta(r - a) \left( \frac{d}{dr} - \frac{B}{r} \right) \quad (6) $$

into the Schrödinger equation. This leads to the Bloch-Schrödinger equation,

$$ \left[ (T_r + \tilde{L} - E) + V(r) \right] u_r^{\text{int}}(r) = \tilde{L} u_r^{\text{ext}}(r). \quad (7) $$

Use of Eq. (4) and Eq. (3) for the radial wave function $u_r(r)$ in Eq. (7) and projecting Eq. (7) on the set of basis states yields at $r = a$

$$ \sum_{j=1}^N [\varphi_j(\tilde{C}(E, B)\varphi_i)] c_j = \frac{\hbar^2}{2\mu} \delta_{i\ell}(a) \left[ a \cdot u_e^{\text{ext}}(a) - B \cdot u_e^{\text{ext}}(a) \right], \quad (8) $$

where $\tilde{C}(E, B)$ is defined by

$$ \tilde{C}(E, B) = T_r + \tilde{L} - E + V(r). \quad (9) $$

It is important to remark that Eq. (8) implies that the solution of Bloch-Schrödinger equation is fully determined by the internal region, while the right-hand side of Eq. (7) contains only values of the channel surface.

### 2.2 Problem of 3-particle channels

The interpretation of Eq. (8) becomes even more striking in the coupled-channel formalism of the R-matrix formalism. The extension of the R-matrix formalism to a coupled-channel system is straightforward and outlined in detail in Ref. [4]. In this formalism Eq. (1) is transformed to a matrix equation

$$ \sum_d \left[ (T_c + E_c - E) + V_{cd} \right] u_d = 0, \quad (10) $$

where $C_c$.
where the indices \( c, d, \ldots \) refer to different channels. Here \( E_c \) is a diagonal matrix and contains for each channel its threshold. Similarly one has to introduce a Bloch operator for each channel of the form

\[
\hat{L}_c = \frac{\hbar^2}{2\mu_c} \delta(r - a_c) \left( \frac{d}{dr} - B_c \right)
\]

in order to restore the hermiticity of the Hamiltonian on \([0, a)\). Projecting the Bloch-Schrödinger equation of the coupled-channel system onto the basis states yields

\[
\sum_d \langle \phi_d | \hat{C}_{cd}(E, B) | \phi_c \rangle c_{d,i} = \sum_d \frac{\hbar^2}{2\mu_d} \phi_d(a)
\]

\[
\times \left[ a \cdot u_d^{\text{ext}}(a) - B_d \cdot u_d^{\text{ext}}(a) \right].
\]

The right-hand side of this equation clearly shows a sum of all involved channel surfaces. For two-body channels all channel surfaces are finite and non-overlapping. Hence a separation in internal and external region is always possible.

Albeit total energy and momentum conservation is also valid in three-body channels there remains freedom in the actual motion of the three bodies. This freedom concerns the mutual directions and the partial kinetic energy of the three collision partners. Thus in a general three-body channel the external region in which no mutual polarization of the bodies occur cannot be fixed in space. Consequently the definition of a finite channel surface for a three-body channel is in general not possible and the formalism of the standard R-matrix theory cannot be applied. In principle one could enlarge the channel surface to include most of the three-body processes, but the feasibility in practice is questionable.

### 3 R-matrix methods for 3-particle channels

#### 3.1 Sequential Approach

In nuclear collisions breakup channels with three outgoing nuclei may occur at rather low energies in the resonance region, especially in light nuclear systems. Therefore the description of breakup channels in R-matrix analyses of such nuclear systems is important. Being aware of the difficulty of R-matrix theory to describe systems with energetically open three- and many-body channels, the possibility of approximations was considered.

In the seminal work of Lane and Thomas [2] the treatment of breakup channels as a succession of two-body disintegrations is worked out. This procedure is applicable if at least two of the three outgoing nuclei form a long-lived compound. In this case the wave function components in all unbound channels are negligible and an approximate finite channel surface can be given. Thus the breakup reaction appears as two successive two-body processes (see Fig. 2).

The procedure has been worked out in detail in Ref. [2]. Here we follow the work of Lane and Thomas [2] and mention only the main difference to the standard treatment. The key for the treatment of successive two-body reactions is the enumeration of the breakup channels. For a given total energy \( E \) the energies \( E_a \) and \( E_b \) are given and consequently we know the energetically open unbound states (labeled by \( r \)) of the long-lived compound \( \beta \). Thus the open states of \( \beta \) are given by \( \psi_{\epsilon(E_a)} \) where the index \( \epsilon \) specifies the composition \((\alpha, \beta)\) of the nuclear system.

The inclusion of the successive breakup is easily implemented by substituting the \( \sum_{\epsilon} \) by \( \sum_{\epsilon} \sum_{\epsilon'} \) \( dE_{\beta} \) in all expressions. Thus the total asymptotic wave function of the system takes the form

\[
\Psi_i - I_i - \sum_{\epsilon'} U_{\epsilon'\epsilon} O_{\epsilon'} = \sum_{\epsilon'} \int dE_{\beta} U_{\epsilon'\epsilon(E_{E_{\beta}})} O_{\epsilon'}.
\]

where the first sum describes the two-body reaction into the composition \((\alpha, \beta)\) and the last sum gives the contribution of the subsequent decay of \( \beta \). Using the collision matrix elements \( U_{\epsilon'\epsilon(E_{E_{\beta}})} \) one can evaluate the cross section of the breakup in the channel \( \epsilon' (E_{E_{\beta}}, r') \) and integrating over all admissible \( E_{\beta} \) and summing over all open channel \( r' \) yields the cross section for given three end products.

#### 3.2 Faddeev equation based R-matrix method

##### 3.2.1 Concept of Faddeev equations

The sequential approach discussed above is a reasonable approximation which is applicable if a long-lived nucleus is involved in the three-body breakup. A quantum mechanically exact treatment of three-body collisions is provided by the Faddeev equations [6]. Therefore Glöckle considered an R-matrix formulation based on the Faddeev equations [3] for three equal masses and \( s \)-states. Unfortunately we did not find any further developments or applications of the method. Therefore an extension of the method to unequal masses was worked out in our group [7].

A three-body problem composed of three nuclei with masses \( m_1, m_2 \) and \( m_3 \) is governed by the total Hamiltonian,

\[
H = \sum_i \frac{p_i^2}{2\mu_i} + \frac{q_i^2}{2\mu_{i,j(k)}} + v_i,
\]

where the indices \( c, d, \ldots \) refer to different channels. Here \( E_c \) is a diagonal matrix and contains for each channel its threshold. Similarly one has to introduce a Bloch operator for each channel of the form

\[
\hat{L}_c = \frac{\hbar^2}{2\mu_c} \delta(r - a_c) \left( \frac{d}{dr} - B_c \right)
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where \( \vec{p}_i \) and \( \vec{q}_i \) are the associated momenta to the Jacobi coordinates \( \vec{r}_i \) and \( \vec{R}_i \), respectively (see Fig. 3).

\[
\begin{align*}
V_i(r_i) & \quad 1(23) \\
V_j(r_j) & \quad 2(31) \\
V_k(r_k) & \quad 3(12)
\end{align*}
\]

Figure 3. Jacobi coordinates and potentials in a three-body system

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\[
\begin{align*}
T & = V + V \hat{g}_0(z) T(z), \\
\hat{g}_0(z) & \text{the free Green's function of the three-body system.}
\end{align*}
\]

\[T(z) = \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} 0 & t_1 & t_1 \\ t_2 & 0 & t_2 \\ t_3 & t_3 & 0 \end{pmatrix} \hat{g}_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix}.
\]

\[
T_i = v_i + v_i \hat{g}_0 T.
\]

Introducing the two-body \( t \)-matrix \( t_i \)

\[t_i = v_i + v_i \hat{g}_0 T_i.
\]

and reformulating Eq. (16) for the components \( T_i \) leads to the uniquely solvable system of Faddeev equations

\[
\begin{align*}
\left( \begin{array}{c} T_1 \\ T_2 \\ T_3 \end{array} \right) = \left( \begin{array}{ccc} t_1 & 0 & t_1 \\ t_2 & 0 & t_2 \\ t_3 & t_3 & 0 \end{array} \right) \hat{g}_0 \left( \begin{array}{c} T_1 \\ T_2 \\ T_3 \end{array} \right).
\end{align*}
\]

For the formulation of the R-matrix method for three-body systems we consider the total scattering wave function \( \Psi^{(s)} \) which is written as sum of three components analogously to the \( T \)-operator

\[
\Psi^{(s)} = \Psi_1(r_1, R_1) + \Psi_2(r_2, R_2) + \Psi_3(r_3, R_3).
\]

3.2.2 Asymptotic breakup amplitude

The asymptotic wave function in the breakup channel is given by the coherent sum of the leading terms of all Faddeev components. Similarly to Ref. [3] we restrict ourselves to a total angular momentum \( L = 0 \), the s-wave part of the potentials \( v_i(r_i) \) and define \( \Psi_i(r_i, R_i) = u_i(r_i, R_i)/(r_i \cdot R_i) \) satisfying the differential equation

\[
\begin{align*}
- \frac{1}{2\mu_{ij}} \frac{d^2}{dr_i^2} - \frac{1}{2\mu_{ij}} \frac{d^2}{dR_i^2} - v_i(r_i) - E u_i(r_i, R_i) \\
&= - \frac{1}{2\mu_{ij}} \int r_i dr_i \sum_{j=1}^3 \int r_{ij} dr_{ij} \frac{u_j(r_j, R_j)}{r_j \cdot R_j}.
\end{align*}
\]

Similarly to [3] we introduce polar coordinates

\[r_i = \sqrt{\frac{1}{2\mu_{ij}}\rho \cos \varphi_i} \quad \text{and} \quad R_i = \sqrt{\frac{1}{2\mu_{ij}}\rho \sin \varphi_i}.
\]

After lengthy calculation and several approximations we find for the asymptotic values of the Faddeev amplitude \( u_i(r_i, R_i) \) in the breakup channel

\[
\begin{align*}
\Psi^{(s)} & \approx 2\mu_{ij} \sqrt{\frac{2}{\pi}} \frac{1}{\rho \rho^{1/2}} \sin \varphi_i T_i \left( \sqrt{\frac{2\mu_{ij}}{\rho^{1/2}}} \cos \varphi_i \right),
\end{align*}
\]

where \( T_i \) are the component \( T \)-operators introduced in (17). Thus the asymptotic breakup amplitude is given by the sum of the three Faddeev components

\[
\Psi^{(s)} = \sum_{i=1}^3 u_i(r_i, R_i) \approx \frac{2\mu_{ij}}{\rho^{1/2}} \sqrt{\frac{2}{\pi}} \frac{1}{\rho \rho^{1/2}} \sin \varphi_i T_i \left( \sqrt{\frac{2\mu_{ij}}{\rho^{1/2}}} \cos \varphi_i \right).
\]

3.2.3 R-matrix formalism for 3-body channels

In order to establish an R-matrix formalism for three-body channels we must introduce an equivalent to the channel surface in two-body channels. We follow the proposal of Glöckle [3] and introduce boarders in the space of Jacobi coordinates given by the contours \( C_1 \) and \( C_2 \).

\[
\begin{align*}
C_1 & : R_i = A_i, \quad 0 \leq r_i \leq a_i, \\
C_2 & : r_i = a_i, \quad 0 \leq R_i \leq A_i.
\end{align*}
\]

Thus a distinction between an inner region \( D \) and external region is the space of Jacobi coordinates \( r_i \) and \( R_i \).
In the internal region $D$ the Faddeev components of the wave functions $u_i(r_i, R_i), i = 1, 2, 3$ are expressed as expansion over a set of linearly independent basis functions $\varphi^{(i)}(r_i, R_i)$.

$$u_i(r_i, R_i) = \sum_{v} \varphi^{(i)}_{v} \varphi^{(i)}(r_i, R_i).$$ (27)

The basis functions are chosen real and orthonormal and are solutions of the differential equation

$$\left[-\frac{1}{2\mu_{jk}} \frac{d^2}{dr_j^2} + v_i(r_i) - \frac{1}{2\mu_{jk}} \frac{d^2}{dR_i^2} - E^{(i)}_v\right] \varphi^{(i)}_v(r_i, R_i) = 0$$ (28)

with the boundary conditions

$$\varphi^{(i)}_v(0, R_i) = \varphi^{(i)}_v(r_i, 0) = \frac{\partial \varphi^{(i)}_v(r_i, R_i)}{\partial R_i} \bigg|_{r_i = 0} = \frac{\partial \varphi^{(i)}_v(r_i, R_i)}{\partial r_i} \bigg|_{R_i = 0} = 0.$$ (29)

Following the proposal of Ref. [3] we use a set of separable basis functions

$$\varphi^{(i)}_v(r_i, R_i) = X^{(i)}_v(r_i) \cdot Y^{(i)}_v(R_i)$$ (30)

which are solutions of the following differential equations

$$\left[-\frac{1}{2\mu_{jk}} \frac{d^2}{dr_j^2} + v_i(r_i) - e_{\nu}\right] X^{(i)}_v(r_i) = 0,$$ (31)

$$\left[-\frac{1}{2\mu_{jk}} \frac{d^2}{dR_i^2} - e_{\nu}\right] Y^{(i)}_v(R_i) = 0.$$ (32)

The eigenenergies of the basis functions $\varphi^{(i)}_v(r_i, R_i)$ are then calculated as $E_v = e_{\nu} + e_{\nu}$. In Fig. 5 we show $X^{(i)}_v(r_i)$ and $Y^{(i)}_v(R_i)$ as an example of basis functions for the system $n^7\text{Be} \rightarrow n + n^4\text{Be}$ considering the subsystem where one neutron is free and $n^4\text{Be}$ form the bound state $^9\text{Be}$ (see Fig. 3). The potential is assumed to be of Woods-Saxon form

$$v_i(r_i) = \frac{v_{0}}{1 + \exp\left(\frac{r_i - r_i^{*}}{b_i}\right)},$$ (33)

with the potential parameters $v_{0} = v_{02} = -13.472$ MeV, $a_1 = a_2 = 0.5$ fm, $b_1 = b_2 = 1.25 \cdot 8^{1/3} = 2.5$ fm and $v_{01} = -50$ MeV, $a_3 = 0.25$ fm, $b_3 = 1.25 \cdot 11^{1/3} = 1.25$ fm.

According to Eq. (27) each Faddeev component is characterized by a certain set of expansion coefficients $c^{(i)}_v$. Matching the internal and the external wave functions and their derivatives at the contours $C_1$ and $C_2$ yields a system of linear equations for the coefficients $c^{(i)}_v$ and the $T$-operator components $T_i$. After some algebra one obtains the system of linear equations (37) together with the set of equations (38) and (39) related to the boundary conditions. The bound and scattering states $u_i^{(+)}(r)$ and $u_i^{(-)}(r)$ of subsystem $(jk)$ are contained in the quantities $M_{ab}$, $M_{jk}$ and $M_{Q0}$ defined in Eq. (34). Together with Eqs. (35) and (36) they enter the system of linear equations,
Solving this system of linear equations numerically yields the various wavenumbers $Q_i$ and $(32)$ at matching radii $r_i$.

4 Summary and conclusions

In this contribution we have briefly revisited the standard R-matrix theory and the problems which arise in the description of three-and many-body channels. We mentioned shortly the key points of the so-called sequential approach [2] which treats the three-body channel as a succession of two two-body reactions. The primary goal of this contribution was the extension of the Faddeev equation based R-matrix formulation of Glöckle [3] to systems with unequal masses with total angular momentum $L = 0$. Albeit the symmetry properties of equal masses are not longer applicable for unequal masses we could derive the asymptotic solutions of the three-body wave functions. Introducing a separation of the Jacobi coordinate space in internal and external regions we could expand the wave function in the internal space with an adequate set of basis functions. Matching the wave functions at the boundary conditions we derived a system of linear equations for the coefficients $c^i_ν$ and the $T$-operator components $T_i$ which are suited for numerical solution. At present the numerical implementation of the algorithm is in progress.

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