

The R -matrix theory

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The R -matrix theory

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Abstract

The different facets of the R -matrix method are presented pedagogically in a general framework. Two variants have been developed over the years: (i) The ‘calculable’ R -matrix method is a calculational tool to derive scattering properties from the Schrödinger equation in a large variety of physical problems. It was developed rather independently in atomic and nuclear physics with too little mutual influence. (ii) The ‘phenomenological’ R -matrix method is a technique to parametrize various types of cross sections. It was mainly (or uniquely) used in nuclear physics. Both directions are explained by starting from the simple problem of scattering by a potential. They are illustrated by simple examples in nuclear and atomic physics. In addition to elastic scattering, the R -matrix formalism is applied to inelastic and radiative-capture reactions. We also present more recent and more ambitious applications of the theory in nuclear physics.

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1. Introduction

1.1. Principle

The R -matrix theory is a powerful tool of quantum physics, introduced by Wigner and Eisenbud [1–3] who simplified an original idea of Kapur and Peierls [4]. The advantage of their simplification is that the R matrix only involves real energy-independent parameters. Initially the theory was aimed at describing resonances in nuclear reactions. However, even the very first developments also contained the principle of a technique for solving coupled-channel Schrödinger equations in the continuum.

At present, the main aim of the R -matrix theory is to describe scattering states resulting from the interaction of particles or systems of particles, which can be nucleons, nuclei, electrons, atoms and molecules. Its principle relies on a division of the configuration space into two regions: the internal and external regions. The boundary between these regions is defined by a parameter known as the channel radius. This radius is chosen large enough so that, in the external region, the different parts of the studied system interact only through known long-range forces and antisymmetrization effects can be neglected. The scattering wave function is approximated there by its asymptotic expression which is known except for some coefficients related to the scattering matrix. In the internal region, the system is considered as confined. Its eigenstates thus form a discrete basis which can be calculated. A scattering wave function at an arbitrary energy is expanded in the internal region over these square-integrable eigenstates. Then, the R matrix, which is the inverse of the logarithmic derivative of the wave function at the boundary, can be calculated. A matching with the solution in the external region provides the scattering matrix. This method can also provide the bound states of the system. In this case, the external solution behaves as a decreasing exponential. Since the exponential decrease depends on the unknown binding energy, an iteration is then necessary.

The R -matrix theory was developed into two different directions with little exchange between these variants. Many of its practitioners often ignore the progress about the other aspect of this double-faced method.

As already mentioned, the original goal was to provide an efficient theory for the treatment of nuclear resonances [3, 5]. From information on bound states and low-energy resonances, it soon became clear that the R -matrix theory offers an efficient way for accurately parametrizing not only resonances but also the non-resonant part of low-energy cross sections with a small number of parameters [5]. An important advantage is that most of these parameters have a physical meaning. This first variant of the method is still very important and much employed, in particular to parametrize the low-energy cross sections relevant in nuclear astrophysics. This version of the R -matrix theory will be called hereafter the phenomenological R matrix. Its properties are reviewed in [5, 6].

The other aspect of the R -matrix theory is that it can provide a simple and elegant way of solving the Schrödinger equation. It is especially competitive in coupled-channel problems with large numbers of open channels where direct

numerical integrations may become unstable. An additional advantage is that narrow resonances which can escape a purely numerical treatment are easily studied. This other facet of the R -matrix theory has been mostly developed in atomic physics although we shall see that it can also be very useful for nuclear-physics applications. This variant will be called hereafter the calculable or computational R matrix. Its properties are reviewed in [7–10].

A very comprehensive review of the phenomenological R -matrix method has been given in 1958 by Lane and Thomas [5]. Their paper contains most of the important aspects of the phenomenological applications of the R matrix to nuclear physics. Many of their results can also be useful for the calculable R matrix. However, in 1957, just before that review appeared in print, an important improvement of the method was published which is therefore not used in their review. Bloch introduced a singular operator defined on the boundary between the two regions, now known as the Bloch operator, which allows a more elegant and compact presentation of the method [11]. The main interest of the Bloch operator is that its use led to extensions of the method to more general treatments of the resolution of the Schrödinger equation in the internal region and opened the way to accurate methods of resolution in atomic and nuclear physics. Several reviews on the computational R matrix have been published in the context of nuclear physics [7] and of atomic physics [8, 10, 12]. Reference [9] deals with both aspects. An update is nevertheless timely.

1.2. The phenomenological R matrix

The phenomenological R matrix and most of its applications were already exhaustively described fifty years ago in [5]. Among these applications, let us mention a detailed study of resonances and an extension of the method to the description of electromagnetic processes. As far as we know, all these applications have been made in nuclear physics, i.e. for the scattering of neutrons on nuclei or of nuclei on nuclei with the presence of a repulsive Coulomb barrier. Nevertheless, using the method still revealed a number of difficulties. In a series of papers, Barker and collaborators provided practical solutions to the determination of the R -matrix parameters from experimental data [13–15] and applied this framework to the spectroscopy and reactions of light nuclei [16, 17]. They also explained non-intuitive effects such as the Thomas–Ehrman shift [17], ghosts of resonances [18] and extended the method to further processes such as radiative-capture reactions [19–21] and delayed β decay [22]. The approach developed by Barker and collaborators has become a standard tool for the analysis of low-energy radiative-capture reactions useful in astrophysics. Recent progress in the adjustment of the R -matrix parameters has been performed in [23, 24].

The R matrix allows parametrizing various physical processes and its determination provides collision matrices and cross sections. For each set of good quantum numbers, i.e. total angular momentum and parity, the dimension of the phenomenological R matrix is equal to the number of channels relevant to the physical properties. When a single channel

is considered, the R matrix for a partial wave with orbital momentum l and total angular momentum J is a function of the energy E parametrized by the formula

$$R_{lJ}(E) = \sum_{n=1}^N \frac{\gamma_{nlJ}^2}{E_{nlJ} - E}. \quad (1.1)$$

In principle, this function possesses an infinity of poles at the real energies E_{nlJ} but only a limited number N of such poles affect the low-energy cross sections. The lowest poles are closely related to bound states at negative energies or to narrow resonances at positive energies. Nevertheless, the poles and the energies of physical states are slightly different. Because of this shift, the determination of these parameters from data requires some skill. The real parameters γ_{nlJ} are known as the reduced width amplitudes because their square is a crucial factor of the width of non-overlapping resonances. More precisely, we shall see in section 3.6 that the width is given as $\Gamma = 2\gamma_{nlJ}^2 P_l$, where P_l is the penetration factor which includes most of the effects of transmission through the Coulomb barrier. This factor depends on energy and the width thus also depends on energy.

A serious drawback of the phenomenological R matrix is that the poles and widths depend on the choice of the channel radius, i.e. on a rather arbitrary value. This aspect of the R matrix has been criticized by a number of authors and has led to further developments of the competing phenomenological K matrix [25]. The K matrix, which provides an alternative formulation of the collision matrix, is also expanded in a series involving an infinity of poles. This approach is based on a delicate treatment of Coulomb functions. In spite of the fact that the K matrix does not contain an arbitrary parameter such as the channel radius, its parametrization is more difficult because its parameters may have a less direct physical interpretation.

1.3. The calculable R matrix

The aim of the calculable R matrix is to provide an efficient way of solving the Schrödinger equation both at positive and negative energies. It was proposed in 1965 by Haglund and Robson and applied to a two-channel problem involving square-well potentials [26]. An expansion over a finite basis was introduced by Buttle [27]. He performed the first realistic application, on $^{12}\text{C} + n$ scattering [27]. He also proposed a correction to the truncation of the R matrix to a finite number of poles, which is now named after him. A more serious problem is a discontinuity of the derivative of the wave function at the boundary between the regions that occurs with the traditional choice of basis states inspired by the original ideas in [3]. Various solutions to the lack of matching at the boundary have been suggested (see [9] for a review). This apparent problem has attracted a lot of attention even long after an efficient technique where it does not occur was introduced [28, 29]. By dropping an unnecessary condition as we will describe, the R -matrix method can be very accurate without matching problems and without need for a Buttle correction.

Some users of the phenomenological R matrix consider the channel radius as a parameter which must be optimized

when fitting the data. Even if this dependence on a parameter without strong physical meaning is weak, this is a drawback that would not be acceptable when aiming at accurately solving the Schrödinger equation. Hence a crucial test of the results of the calculable R matrix is an almost perfect independence with respect to the choice of channel radius. This test provides a measure of the accuracy of the calculations.

In spite of its introduction for nuclear-physics problems [26, 27], this approach was first extensively developed to study electron (or positron) collisions on atoms and molecules [8, 10, 12]. It allows describing of the excitation and ionization of these systems. Photoionization, i.e. collisions with a photon leading to the single or double ionization of the atom, is also a well-studied application [30, 31].

Important and difficult aspects of these atomic-physics problems are the non-locality of the interaction due to electron exchanges and the long-range nature of the interactions, due to the polarization interactions. The non-locality is well treated in the R -matrix approach. The long range of the force implies that the asymptotic behaviour of the solution is only reached for very large values of the interparticle distance. To avoid using a very large channel radius, propagation methods have been introduced [32]. They involve an intermediate region where the interaction can be simplified, for example with an asymptotic expansion.

Electron scattering on heavy atoms has required the introduction of relativistic corrections. The extension of the R matrix to the Dirac equation was introduced as early as in 1948 [33] but its validity remained controversial for a long time. Relativistic corrections were thus first derived from the Breit–Pauli equation. The validity of the Dirac extension is now well established and elaborate relativistic codes have been developed. This aspect will not be covered here (see [34] for a recent review).

In nuclear physics, the computational R matrix is much less used although it should be very useful in large coupled-channel calculations. It has been much applied in microscopic cluster calculations in which the difficult antisymmetrization is taken into account in the internal region only [35, 36]. The versatility of the R matrix found interesting applications in processes where bound and scattering states are mixed, such as radiative capture or delayed β decay [37, 38]. The application of the R -matrix method to coupled-channel calculations has been simplified by its combination with the Lagrange-mesh method which avoids calculating matrix elements of the potentials [39–41]. Recently, this approach has been extended to non-local interactions [42].

Other approaches to the same problem present a number of similarities. The variational K -matrix method [43] has a very similar spirit. The Kohn variational principle for the logarithmic derivative is equivalent to the calculable R matrix [44]. Practical implementations of the Gamow-state method [45] are also exactly equivalent to the R -matrix calculations [46].

1.4. Outline

In this review, we present both calculable and phenomenological versions of the R -matrix theory. Very few papers

deal with both aspects simultaneously [47, 48]. Since many excellent reviews already exist, we try to make an introductory presentation, illustrated with simple numerical examples. We also show the parallel evolutions of the method in atomic and nuclear physics and try to shed light on some common misunderstandings or controversies about the R -matrix methods. The numerical examples that we display are tailored to allow a motivated reader to test his/her understanding by reproducing them with limited effort. Because of our background as nuclear physicists, most examples (but not all) correspond to nuclear applications. Finally, we also review state-of-the-art calculations in nuclear physics where the R matrix proves useful.

Contrary to tradition, we start with the calculable R matrix on a finite basis, which provides a convenient numerical approach. Taking the limit for an infinite complete basis will introduce the theoretical R matrix which leads after truncation to the phenomenological approximation (1.1). For the sake of simplicity, we detail potential scattering in the single-channel case so avoiding the unpedagogical definitions of channel wave functions. We only provide the main steps for the multichannel case.

The bibliography about the R matrix is enormous and cannot be fully covered here. We have tried to quote papers that we think significant or useful for further bibliographic research.

In section 2, we introduce the necessary basics of scattering theory with radiative capture as a more elaborate application. The calculable R matrix is presented in section 3 and relatively simple numerical applications in section 4. The phenomenological R matrix and its applications are presented in section 5. Recent elaborate calculations in nuclear physics are reviewed in section 6. Concluding remarks are made in section 7.

2. Summary of scattering theory

2.1. Coulomb scattering

Consider the collision of two particles with respective masses m_1 and m_2 and charges Z_1e and Z_2e at a positive energy E in the centre-of-mass frame. The wavenumber is defined as

$$k = \sqrt{2\mu E}/\hbar, \quad (2.1)$$

where $\mu = m_1m_2/(m_1 + m_2)$ is the reduced mass.

Let us start with some definitions about pure Coulomb scattering. In this case, a Bohr radius can be defined as

$$a_B = \frac{\hbar^2}{\mu|Z_1Z_2|e^2}. \quad (2.2)$$

A useful parameter is the dimensionless Sommerfeld parameter

$$\eta = \frac{Z_1Z_2e^2}{\hbar v} = \frac{\text{sgn}(Z_1Z_2)}{a_B k}, \quad (2.3)$$

where $v = \hbar k/\mu$ is the relative velocity. Parameter η measures the importance of Coulomb effects at a given energy. The neutral case is recovered with $\eta = 0$.

For a central potential, a wave function can be factorized in spherical coordinates $\mathbf{r} = (r, \Omega)$ as $\psi(\mathbf{r}) = r^{-1}u_l(r)Y_l^m(\Omega)$. The spherical harmonics $Y_l^m(\Omega)$ depend on the orbital and magnetic quantum numbers l and m , and on the angles $\Omega = (\theta, \varphi)$. They are defined according to the convention of Condon and Shortley. The radial Schrödinger equation for the Coulomb problem in partial wave l then reads

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2k\eta}{r} + k^2 \right) u_l(r) = 0. \quad (2.4)$$

Its solutions are combinations of the regular and irregular Coulomb functions $F_l(\eta, kr)$ and $G_l(\eta, kr)$ [49]. The regular function vanishes at the origin and is normalized at infinity according to

$$F_l(\eta, x) \xrightarrow{x \rightarrow \infty} \sin\left(x - \frac{1}{2}l\pi - \eta \ln 2x + \sigma_l\right), \quad (2.5)$$

where appears the Coulomb phase shift

$$\sigma_l = \arg \Gamma(l+1+i\eta) \quad (2.6)$$

involving the Euler function Γ . The irregular function $G_l(\eta, x)$ is unbound at the origin (except for $\eta = l = 0$) and is fixed by its asymptotic behaviour

$$G_l(\eta, x) \xrightarrow{x \rightarrow \infty} \cos\left(x - \frac{1}{2}l\pi - \eta \ln 2x + \sigma_l\right). \quad (2.7)$$

Also very useful are the conjugate functions

$$I_l(\eta, x) = G_l - iF_l, \quad O_l(\eta, x) = G_l + iF_l, \quad (2.8)$$

which behave asymptotically like incoming and outgoing waves, respectively,

$$\begin{aligned} I_l(\eta, x) &\xrightarrow{x \rightarrow \infty} e^{-i(x - \frac{1}{2}l\pi - \eta \ln 2x + \sigma_l)}, \\ O_l(\eta, x) &\xrightarrow{x \rightarrow \infty} e^{i(x - \frac{1}{2}l\pi - \eta \ln 2x + \sigma_l)}. \end{aligned} \quad (2.9)$$

Note that we do not follow here the same phase convention as Lane and Thomas [5]. In the neutral case, one has $F_l(0, x) = x j_l(x)$ and $G_l(0, x) = x n_l(x)$ where j_l and $n_l = -y_l$ are spherical Bessel functions [49].

In some applications, solutions of (2.4) are also needed at negative energies. The real solution decreasing at infinity is the Whittaker function $W_{-\eta_B, l+\frac{1}{2}}(2\kappa_B r)$ [49]. It depends on the wave number $\kappa_B = \sqrt{-2\mu E}/\hbar$ and on the Sommerfeld parameter $\eta_B = \text{sgn}(Z_1Z_2)/a_B\kappa_B$ of the bound state. Whittaker functions behave asymptotically as

$$W_{-\eta_B, l+\frac{1}{2}}(x) \xrightarrow{x \rightarrow \infty} x^{-\eta_B} e^{-x/2}. \quad (2.10)$$

They are singular at the origin.

A bounded solution of the three-dimensional Schrödinger equation at a positive energy with the same Coulomb potential is given by [50]

$$\begin{aligned} \psi_C^+(r) &= (2\pi)^{-3/2} e^{-\pi\eta/2} \Gamma(1+i\eta) e^{ikz} {}_1F_1(-i\eta, 1, ik(r-z)), \\ &\quad (2.11) \end{aligned}$$

where ${}_1F_1$ is the confluent hypergeometric function [49]. This wave function has the asymptotic behaviour of an outgoing scattering state

$$\psi_C^+(r) \xrightarrow{|r-z| \rightarrow \infty} (2\pi)^{-3/2} \left(e^{i[kz + \eta \ln k(r-z)]} + f_C(\Omega) \frac{e^{i(kr - \eta \ln 2kr)}}{r} \right). \quad (2.12)$$

The coefficient of the second term is the Coulomb scattering amplitude,

$$f_C(\Omega) = -\frac{\eta}{2k \sin^2 \frac{1}{2}\theta} e^{2i(\sigma_0 - \eta \ln \sin \frac{1}{2}\theta)}. \quad (2.13)$$

The square of the modulus of f_C provides the Rutherford cross section. Function ψ_C^+ can be expanded in partial waves as

$$\psi_C^+(r) = (2\pi)^{-3/2} (kr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^l e^{i\sigma_l} P_l(\cos \theta) F_l(\eta, kr), \quad (2.14)$$

where P_l is a Legendre polynomial [49].

2.2. Scattering by a potential

Consider a potential V tending to the Coulomb potential faster than r^{-2} ,

$$V(r) \xrightarrow{r \rightarrow \infty} \frac{Z_1 Z_2 e^2}{r} + o\left(\frac{1}{r^2}\right). \quad (2.15)$$

The radial Schrödinger equation in partial wave l reads

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu V(r)}{\hbar^2} + k^2 \right) u_l(r) = 0 \quad (2.16)$$

with the condition at the origin

$$u_l(0) = 0. \quad (2.17)$$

A real solution at positive energy E behaves asymptotically as

$$u_l(r) \xrightarrow{r \rightarrow \infty} \cos \delta_l F_l(\eta, kr) + \sin \delta_l G_l(\eta, kr), \quad (2.18)$$

up to a normalization factor. The important physical quantity is the phase shift δ_l . For later use, it is however more convenient to write the solution as

$$u_l(r) \xrightarrow{r \rightarrow \infty} C_l [I_l(\eta, kr) - U_l O_l(\eta, kr)], \quad (2.19)$$

where C_l can be chosen in various ways. For example, (2.18) is recovered with $C_l = i \exp(-i\delta_l)/2$ and the normalization of the u_l with respect to $\delta(k - k')$ is obtained with $C_l = i \exp(-i\delta_l)/\sqrt{2\pi}$. The collision or scattering ‘matrix’ U_l is given by

$$U_l = e^{2i\delta_l}. \quad (2.20)$$

With the different partial solutions, one can construct an outgoing stationary solution

$\Psi^+(r)$

$$= (2\pi)^{-3/2} (2kr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^{l+1} e^{i\sigma_l} P_l(\cos \theta) C_l^{-1} u_l(r) \quad (2.21)$$

behaving asymptotically as a Coulomb wave (2.11) propagating in the z direction plus an outgoing spherical wave

$$\Psi^+(r) \xrightarrow{r \rightarrow \infty} \psi_C^+(r) + (2\pi)^{-3/2} f(\Omega) \frac{e^{i(kr - \eta \ln 2kr)}}{r}. \quad (2.22)$$

The coefficient of the second term in this asymptotic expression determines the additional scattering amplitude

$$f(\Omega) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) e^{2i\sigma_l} (U_l - 1) P_l(\cos \theta). \quad (2.23)$$

From (2.23), one obtains the elastic cross section

$$\frac{d\sigma}{d\Omega} = |f_C(\Omega) + f(\Omega)|^2 \quad (2.24)$$

also involving the Coulomb amplitude (2.13). The scattering wave function (2.21) is useful in various types of reactions. We illustrate it below with radiative capture.

2.3. Collisions in a many-body system

An N -body system is described with the microscopic Hamiltonian

$$H = T + V = \sum_{i=1}^N T_i + \sum_{i>j=1}^N V_{ij}, \quad (2.25)$$

where for simplicity we only display two-body forces. This Hamiltonian is invariant under rotations, translations and reflections. We do not display nor discuss the removal of the centre of mass.

At positive excitation energies, several channels may be open. In each channel, the particles are divided into various groups. Each such division is known as a partition. A given partition is denoted as α . For simplicity, we only consider here channels where the particles form only two subsystems: $N = N_\alpha^{(1)} + N_\alpha^{(2)}$. Both subsystems of partition α are described with an internal Hamiltonian $H_\alpha^{(i)}$ ($i = 1, 2$) which has the form (2.25) with N replaced by $N_\alpha^{(i)}$.

A channel c is defined by specifying in addition the energy of each subsystem, i.e. a certain eigenvalue for each internal Hamiltonian. The exact or approximate energies $E_c^{(i)}$ and wave functions $\phi_c^{(i)}$ are related by

$$E_c^{(i)} = \langle \phi_c^{(i)} | H_c^{(i)} | \phi_c^{(i)} \rangle. \quad (2.26)$$

Here and in what follows, subscript c has a variable symbolic meaning depending on the considered quantity. In $H_c^{(i)} \equiv H_\alpha^{(i)}$, it represents the set of internal coordinates of subsystem i . In $E_c^{(i)}$, it represents a set of quantum numbers. In $\phi_c^{(i)}$, it means both. When $\phi_c^{(i)}$ is not an exact eigenfunction of $H_c^{(i)}$, (2.26) remains valid from a variational perspective.

To each partition α of the system into two subsystems may correspond several channels differing by their internal states. Each channel c has a threshold energy

$$E_c = E_c^{(1)} + E_c^{(2)} \quad (2.27)$$

defined with respect to some common reference energy. A channel is open or closed according to whether E_c is smaller or larger than the total energy E of the system. In each open channel, one can define a wave number $k_c = \sqrt{2\mu_c(E - E_c)}/\hbar$ and a relative velocity $v_c = \hbar k_c/\mu_c$, μ_c being the reduced mass of partition α . In each closed channel, one can define a wave number $\kappa_c = \sqrt{2\mu_c(E_c - E)}/\hbar$.

For each partition α , the relative coordinate $\mathbf{r}_c \equiv \mathbf{r}_\alpha$ is the difference between the centre-of-mass coordinates of the subsystems. The eigenstates of each subsystem $i = 1, 2$ are characterized by their energy $E_c^{(i)}$ and by their good quantum numbers, i.e. the total angular momentum I_i (usually called spin) and its projection M_i . Under the time reversal operator K [50], they are assumed to transform according to the convention

$$K|JM\rangle = (-1)^{J-M}|J-M\rangle. \quad (2.28)$$

A channel state is an eigenstate of the total angular momentum of the full system resulting from the coupling of both internal states $\phi_{cI_1M_1}^{(1)}$ and $\phi_{cI_2M_2}^{(2)}$ with a spherical harmonics depending on the angles Ω_c defining the orientation of the relative coordinate \mathbf{r}_c . More precisely, a channel state is represented as

$$|c\rangle = i^{l_c} [[\phi_{cI_1}^{(1)} \otimes \phi_{cI_2}^{(2)}]_{I_c} \otimes Y_{l_c}(\Omega_c)]^{JM\pi}, \quad (2.29)$$

where I_c is the channel spin resulting from the coupling of I_1 and I_2 , l_c is the orbital momentum of the relative motion in channel c , J is the total angular momentum quantum number of the many-body system, M is its projection and π is the total parity. Thanks to the phase factor i^{l_c} , the channel states transform under time reversal according to (2.28). For simplicity, we do not display the parity quantum numbers π_{c1} and π_{c2} of the subsystems. They are related to the total parity by

$$\pi = \pi_{c1}\pi_{c2}(-1)^{l_c}. \quad (2.30)$$

Channel states are assumed orthogonal to each other and normed,

$$\langle c|c'\rangle = \delta_{cc'}. \quad (2.31)$$

The orthogonality is not obvious for different partitions α and α' . In that case, it is only true asymptotically.

Since Hamiltonian H is invariant under rotation and reflection, J , M and π are good quantum numbers. A partial wave of the total wave function of the system at energy E can be written as

$$\Psi_{(c_0)}^{JM\pi} = \sum_c \mathcal{A}|c\rangle r_c^{-1} u_{c(c_0)}(r_c), \quad (2.32)$$

where indices c_0 and c may represent either all quantum numbers appearing (or understood) in the right-hand side of (2.29) or a relevant subset of them. Projector \mathcal{A} performs any antisymmetrization due to the indistinguishability of some identical particles. These can be electrons in atomic physics or nucleons in nuclear physics within the isospin formalism. The subscript (c_0) recalls the entrance channel as explained below. This wave function is an approximate eigenstate of the full many-body Hamiltonian

$$H\Psi_{(c_0)}^{JM\pi} = E\Psi_{(c_0)}^{JM\pi}. \quad (2.33)$$

To complete the definition of $\Psi_{(c_0)}^{JM\pi}$, one must specify its asymptotic behaviour.

We shall describe the asymptotic behaviour in terms of the collision or scattering matrix which is usually denoted as U in the R -matrix context. This matrix is interesting physically because it is directly related to cross sections but it leads to complex radial wave functions. Calculations only involving real radial wave functions are also possible (for real potentials). They are dominantly used in atomic physics [51] but are also encountered in nuclear physics [9]. The relation between both approaches is summarized in [appendix A](#).

The asymptotic behaviour in open channels generalizing (2.19) is given by

$$u_{c(c_0)}(r_c) \xrightarrow{r_c \rightarrow \infty} C_{c_0} v_c^{-1/2} [\delta_{cc_0} I_c(k_c r_c) - U_{cc_0} O_c(k_c r_c)]. \quad (2.34)$$

In (2.34), I_c and O_c are defined as in (2.8) and C_{c_0} is arbitrary (see [appendix A](#)). The asymptotic form is chosen in such a way that incoming flux only occurs in the entrance channel c_0 . Taking all possible entrance channels c_0 into account, the coefficients U_{cc_0} of the outgoing waves form the collision matrix U . It is defined for each angular momentum J and parity π . Its dimension is given by the number of open channels at energy E . Closed channels may also appear in expansion (2.32) but the asymptotic behaviour of the corresponding radial functions is exponentially decreasing according to (2.10).

For real potentials, thanks to the introduction of coefficients $v_c^{-1/2}$, current conservation imposes that the collision matrix is unitary,

$$UU^\dagger = U^\dagger U = \mathbf{1}. \quad (2.35)$$

Because of time-reversal invariance, it is also symmetric,

$$U = U^T, \quad (2.36)$$

where T means transposition. This property imposes the phase i^{l_c} in definition (2.29) of the channel states. As shown by Huby [52], this factor is missing in some important references [3, 53] and some phases must be corrected accordingly. This correction is not necessary if the symmetry property (2.36) is never used. A matrix with properties (2.35) and (2.36) can be diagonalized with an orthogonal (real) matrix S ,

$$S^T U S = e^{2i\delta}, \quad (2.37)$$

where δ is a diagonal matrix whose elements are the eigenphases δ_n .

Introducing (2.32) in the Schrödinger equation (2.33) and projecting over a channel wave function $|c\rangle$ leads to the coupled equations

$$\begin{aligned} [T_c + V_c(r) + E_c - E] u_{c(c_0)}(r) \\ + \sum_{c'} \int_0^\infty W_{cc'}(r, r') u_{c'(c_0)}(r') dr' = 0. \end{aligned} \quad (2.38)$$

They involve the kinetic-energy operators

$$T_c = -\frac{\hbar^2}{2\mu_c} \left(\frac{d^2}{dr^2} - \frac{l_c(l_c + 1)}{r^2} \right). \quad (2.39)$$

The local or direct potentials are defined by

$$V_c(r_c) = \langle c|V|c \rangle, \quad (2.40)$$

where V is the total potential appearing in the many-body Hamiltonian (2.25) and the integration is performed over the internal coordinates of the subsystems appearing in channel c . The non-local potentials

$$W_{cc'}(r, r') = \langle c|\delta(r_c - r)V\mathcal{A}\delta(r_{c'} - r')|c' \rangle - V_c(r)\delta_{cc'}\delta(r - r') \quad (2.41)$$

occur because of antisymmetrization and/or because several partitions are taken into account.

Mathematically, system (2.38) can be written as a function of a single coordinate r (which becomes r' in the integrals of the non-local terms). Wave functions, however, depend on several relative coordinates r_c when several partitions are taken into account. Channels c differ either by the nature of the subsystems or by their level of excitation. To simplify the presentation, we now consider that a single partition is taken into account or that all coordinates r_c are approximated by a single one. Interactions may still be non-local but this does not raise major problems as long as the non-local terms are short-ranged.

The colliding systems have initial orientations specified by the spin projections M_1 and M_2 in the entrance channel now denoted as c . One is looking for a solution of the Schrödinger equation with the asymptotic behaviour

$$\begin{aligned} \Psi_{(cM_1M_2)}^+(\mathbf{r}) &\xrightarrow{r \rightarrow \infty} \psi_C^+(\mathbf{r})\phi_{cI_1M_1}^{(1)}\phi_{cI_2M_2}^{(2)} \\ &+ (2\pi)^{-3/2} \sum_{c'M_1M_2'} \frac{e^{i(k_{c'}r - \eta_{c'} \ln 2k_{c'}r)}}{r} f_{c'M_1M_2'}^{(cM_1M_2)}(\Omega) \phi_{c'I_1M_1'}^{(1)}\phi_{c'I_2M_2'}^{(2)}. \end{aligned} \quad (2.42)$$

Several scattering amplitudes $f_{c'M_1M_2'}^{(cM_1M_2)}$ appear. The partial wave functions (2.32) read with $|c\rangle$ representing $|\alpha I_1 I_2\rangle I J M\rangle$,

$$\Psi_{(c)}^{JM\pi}(\mathbf{r}) = \sum_{c'} |c'\rangle r^{-1} u_{c'(c)}(r). \quad (2.43)$$

A stationary scattering wave function is constructed as

$$\begin{aligned} \Psi_{(cM_1M_2)}^+(\mathbf{r}) &= i(2\pi)^{-3/2} \pi^{1/2} k^{-1} \sum_{J\pi} \sum_{I\ell} C_c^{-1} (2\ell + 1)^{1/2} e^{i\sigma_I} \\ &\times (I_1 I_2 M_1 M_2 | I M) (I \ell M 0 | J M) \Psi_{(c)}^{JM\pi}(\mathbf{r}) \end{aligned} \quad (2.44)$$

with $M = M_1 + M_2$. From the outgoing waves of the asymptotic form of (2.44), one deduces the scattering amplitudes

$$\begin{aligned} f_{c'M_1M_2'}^{(cM_1M_2)}(\Omega) &= i \frac{\sqrt{\pi}}{k} \sum_{J\pi} \sum_{I\ell} \sum_{I'\ell'} (2\ell + 1)^{1/2} e^{i(\sigma_I + \sigma_{I'})} (I_1 I_2 M_1 M_2 | I M) \\ &\times (I \ell M 0 | J M) (I_1' I_2' M_1' M_2' | I' M') (I' \ell' M' M - M' | J M) \\ &\times (\delta_{c'c} \delta_{I'I'} \delta_{\ell'\ell} - U_{c'I'I',cII}^{J\pi}) Y_{\ell'}^{M-M'}(\Omega), \end{aligned} \quad (2.45)$$

where $M' = M_1' + M_2'$. The elastic cross section averaged over initial orientations and summed over final orientations reads

$$\begin{aligned} \frac{d\sigma_{\text{el.}}}{d\Omega} &= \frac{1}{(2I_1 + 1)(2I_2 + 1)} \\ &\times \sum_{M_1M_2} \sum_{M_1'M_2'} |f_C(\Omega) \delta_{M_1'M_1} \delta_{M_2'M_2} + f_{cM_1'M_2'}^{(cM_1M_2)}(\Omega)|^2, \end{aligned} \quad (2.46)$$

where f_C is defined in (2.13). Inelastic or reaction cross sections are given by

$$\frac{d\sigma_{c \rightarrow c'}}{d\Omega} = \frac{1}{(2I_1 + 1)(2I_2 + 1)} \sum_{M_1M_2} \sum_{M_1'M_2'} |f_{c'M_1'M_2'}^{(cM_1M_2)}(\Omega)|^2 \quad (2.47)$$

for $c' \neq c$. The summations can be performed analytically. A long but simple calculation provides [53]

$$\frac{d\sigma_{c \rightarrow c'}}{d\Omega} = \frac{\pi}{k^2} \frac{1}{(2I_1 + 1)(2I_2 + 1)} \sum_{\lambda} B_{\lambda}(E) P_{\lambda}(\cos \theta), \quad (2.48)$$

where the anisotropy coefficients $B_{\lambda}(E)$ are given by

$$\begin{aligned} B_{\lambda}(E) &= \frac{1}{4\pi} \sum_{J\pi} \sum_{I\ell} \sum_{J'\pi'} \sum_{I'\ell'} (-1)^{I-I'} e^{i(\sigma_I + \sigma_{I'} - \sigma_{\ell} - \sigma_{\ell'})} Z(I J L J', I \lambda) \\ &\times Z(I' J' L' J', I' \lambda) U_{c'I'I',cII}^{J\pi}(E) U_{c'I'L',cIL}^{J'\pi'^*}(E). \end{aligned} \quad (2.49)$$

The real coefficients Z defined in [53] are modified here for consistency with the symmetry property (2.36) of the collision matrix as [52]

$$\begin{aligned} Z(I J L J', I \lambda) &= (-1)^{J+J'} [(\lambda + 1)(2J + 1)(2J' + 1)(2\ell + 1)(2L + 1)]^{1/2} \\ &\times \begin{pmatrix} \ell & L & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell & L & \lambda \\ J' & J & I \end{Bmatrix}. \end{aligned} \quad (2.50)$$

They verify the symmetry relation

$$Z(I J L J', I \lambda) = Z(L J' I J, I \lambda). \quad (2.51)$$

From B_0 , one deduces the integrated inelastic or reaction cross sections

$$\begin{aligned} \sigma_{c \rightarrow c'} &= \frac{\pi}{k^2} \frac{1}{(2I_1 + 1)(2I_2 + 1)} \sum_{J\pi} (2J + 1) \sum_{I\ell} \sum_{I'\ell'} |U_{c'I'I',cII}^{J\pi}(E)|^2. \end{aligned} \quad (2.52)$$

For the elastic cross section, the summation over the orientations can also be performed analytically [53] and provides three contributions: nuclear and Coulomb cross sections, as well as an interference term. However, in practical applications, it turns out that definition (2.46) is more direct to use.

2.4. Radiative capture

In nuclear physics, radiative capture is an important process because of its astrophysical applications [54]. In this reaction, the two colliding nuclei fuse into a nucleus with mass m with the emission of a photon. In stars, this process often occurs at very low scattering energies and requires that the reaction has a positive threshold energy $Q = (m_1 + m_2 - m)c^2$. The analogue reaction in atomic physics is electron capture. However, much more attention is paid in that field to the reversed process, namely photoionization. Here we shall proceed with radiative capture in a nuclear physics context but the formulae can be easily adapted to photodissociation or to photoionization by using the detailed balance.

Radiative capture is an electromagnetic transition from a scattering state to a bound state. The electromagnetic aspects of this process can be studied at first order of perturbation theory [5], with an outgoing scattering state $\Psi_{(cM_1M_2)}^+$ as initial state at positive energy E and a bound state in partial wave $J_f\pi_f$ as final state at negative energy E_f . The final energy E_f is equal to $-Q + E_x$ where E_x is the excitation energy of the final level with respect to the ground state. The radiative-capture cross section to this state is then given by

$$\sigma_{J_f\pi_f}(E) = \frac{64\pi^4}{\hbar v} \frac{1}{(2I_1 + 1)(2I_2 + 1)} \sum_{\sigma\lambda} \frac{k_\gamma^{2\lambda+1}}{[(2\lambda + 1)!!]^2} \frac{\lambda + 1}{\lambda} \times \sum_{M_1M_2M_f\mu} |\langle \Psi_{J_fM_f\pi_f} | \mathcal{M}_\mu^{\sigma\lambda} | \Psi_{(cM_1M_2)}^+(E) \rangle|^2, \quad (2.53)$$

where the symbols $\sigma\lambda$ label the electric ($E\lambda$) and magnetic ($M\lambda$) multipoles and the corresponding multipole operators are denoted as $\mathcal{M}_\mu^{\sigma\lambda}$ ($\mu = -\lambda, +\lambda$) [55]. The photon wave number is given by

$$k_\gamma = (E - E_f)/\hbar c. \quad (2.54)$$

In practice, the sum over $\sigma\lambda$ can usually be restricted to the dominant electric multipole ($E1$, or $E2$ when $E1$ is forbidden) because k_γ is small with respect to the inverse of the nucleus dimension. Below the Coulomb barrier, the cross section strongly depends on energy. To reduce the energy dependence, it is often converted into the astrophysical S -factor, defined as

$$S_{J_f\pi_f}(E) = E \exp(2\pi\eta) \sigma_{J_f\pi_f}(E), \quad (2.55)$$

where η is the Sommerfeld parameter.

Let us restrict the scattering wave function to a single channel. The spins I_1 and I_2 are then fixed and only I and l are needed to specify the entrance channel. By using expansion (2.44) in this particular case, the cross section (2.53) can be written as

$$\sigma_{J_f\pi_f}(E) = \sum_{\sigma\lambda} \sigma_{J_f\pi_f}^{\sigma\lambda}(E), \quad (2.56)$$

where the partial cross section of multipolarity $\sigma\lambda$ reads, in analogy with (2.52),

$$\sigma_{J_f\pi_f}^{\sigma\lambda}(E) = \frac{\pi}{k^2} \frac{1}{(2I_1 + 1)(2I_2 + 1)} \times \sum_{J\pi} (2J + 1) \sum_{II} |\tilde{U}_{II}^{\sigma\lambda}(E, J\pi \rightarrow J_f\pi_f)|^2. \quad (2.57)$$

In (2.57), $\tilde{U}_{II}^{\sigma\lambda}$ is dimensionless and proportional to a matrix element of the electromagnetic operator between the final state and the initial partial wave. From (2.44) and (2.53), it is given by

$$\tilde{U}_{II}^{\sigma\lambda}(E, J\pi \rightarrow J_f\pi_f) = \left(\frac{2J_f + 1}{2J + 1} \right)^{1/2} \left(\frac{8\pi(\lambda + 1)k_\gamma^{2\lambda+1}}{\hbar v \lambda (2\lambda + 1)!!^2} \right)^{1/2} \times \frac{1}{C_{II}} \langle \Psi_{J_f\pi_f} | \mathcal{M}^{\sigma\lambda} | \Psi_{(II)}^J(E) \rangle, \quad (2.58)$$

where the reduced matrix element is defined by

$$\langle \Psi_{J_fM_f\pi_f} | \mathcal{M}_\mu^{\sigma\lambda} | \Psi_{(II)}^{JM\pi} \rangle = (J\lambda M\mu | J_fM_f) \langle \Psi_{J_f\pi_f} | \mathcal{M}^{\sigma\lambda} | \Psi_{(II)}^J \rangle. \quad (2.59)$$

For a number of reactions involving light nuclei, capture mainly occurs at distances where the wave functions of the colliding nuclei overlap weakly. This situation can be described by a simple model where the internal structure of the colliding nuclei is neglected and the physics of the process is modelled by a local potential V depending on the distance r between the centres of mass of the nuclei. In this case, the asymptotic form of the initial state is described by (2.42) where the internal states $\phi_{cI_1M_1}^{(1)}$ and $\phi_{cI_2M_2}^{(2)}$ reduce to spinors $|I_1M_1\rangle$ and $|I_2M_2\rangle$.

The electric operators $\mathcal{M}_\mu^{E\lambda}$ are given in this simple model by

$$\mathcal{M}_\mu^{E\lambda} = e Z_{\text{eff}}^{(E\lambda)} r^\lambda Y_\lambda^\mu(\Omega), \quad (2.60)$$

where $Z_{\text{eff}}^{(E\lambda)}$ is the effective charge

$$Z_{\text{eff}}^{(E\lambda)} = Z_1 \left(-\frac{m_2}{m} \right)^\lambda + Z_2 \left(\frac{m_1}{m} \right)^\lambda. \quad (2.61)$$

The radiative-capture cross section to a final bound state with angular momentum J_f can be calculated in this model. The initial scattering state with quantum numbers JM is defined by (2.44) where (2.43) is replaced by

$$\Psi^{JM}(r) = \sum_{II} i^l |(I_1I_2)IIJM\rangle r^{-1} u_{II}^J(r) \quad (2.62)$$

and radial functions are normalized according to (2.34). The normed final bound state with quantum numbers J_fM_f is assumed to be approximated by expression (2.62) with the normalization

$$\sum_{I_fI_f} \int_0^\infty [u_{I_fI_f}^{J_f}(r)]^2 dr = 1. \quad (2.63)$$

The reduced matrix element reads

$$\langle \Psi_{J_f\pi_f} | \mathcal{M}^{E\lambda} | \Psi_{(II)}^{JM\pi}(E) \rangle = e Z_{\text{eff}}^{(E\lambda)} [4\pi(2J_f + 1)]^{-1/2} \times \sum_{I_fI_f} (-1)^{I_f-J} Z(I_fJ_fI_fJ, I_f\lambda) \int_0^\infty u_{I_fI_f}^{J_f}(r) r^\lambda u_{I_fI_f}^J(r) dr. \quad (2.64)$$

In practice, (2.64) must often be corrected empirically by multiplicative factors called spectroscopic factors to take an approximate account of the internal structure of the nuclei [56].

3. The calculable R matrix

3.1. Introduction

The two variants of the R matrix method mainly differ by their types of applications. In the calculable R matrix, the aim is to accurately solve a given Schrödinger equation mostly in the continuum, i.e. for positive energies. In the phenomenological R matrix, the goal is to parametrize scattering data; it is thus essential to know the analytical form of the R matrix. Of course, both variants have much in common and it is a matter of taste to start with one or the other. Historically, in nuclear physics, the emphasis has first been put on the phenomenological variant. Conversely, most applications in atomic physics are related to the calculable R matrix. Here we will start with a general formalism leading to the calculable version and then deduce the properties allowing the phenomenological use.

First, we restrict ourselves to a single channel for an arbitrary partial wave. This assumption is often valid, and allows simple notations. We thus attempt to find approximate solutions of the Schrödinger equation for the relative motion of two particles with reduced mass μ interacting via a central potential V . At large relative distances r , the interaction reduces to the Coulomb interaction V_C .

After separation of the angular part, the radial Schrödinger equation (2.16) for partial wave l can be written as

$$(H_l - E)u_l = 0. \quad (3.1)$$

In this expression, the radial Hamiltonian H_l is defined as

$$H_l = T_l + V(r), \quad (3.2)$$

where T_l is given by (2.39). We are interested in bounded solutions $u_l(r)$ of (3.1) verifying condition (2.17) at the origin. Bound-state solutions at negative energies are square integrable over $(0, \infty)$ and can be normed. Scattering solutions at positive energies are assumed to be normalized according to (2.19) with the scattering matrix U_l defined in (2.20). We will essentially deal with real potentials for which the phase shifts are real and the scattering matrix is unitary. The generalization to complex potentials is straightforward.

3.2. Definition and calculation of the R matrix

In the R -matrix method, the configuration space is divided at the channel radius a into an internal region and an external region. The channel radius is chosen large enough so that V can be approximated by V_C in the external region at the required accuracy. This means that the channel radius can in principle always be increased although often at a cost of computational time. At each energy E , the wave function is defined by different expressions in these regions. In the external region, the wave function $u_l(r)$ is approximated by the exact asymptotic expression (2.19)³,

$$u_l^{\text{ext}}(r) = C_l[I_l(kr) - U_l O_l(kr)]. \quad (3.3)$$

³ From now on, the Sommerfeld parameter η is implied.

In the internal region, the wave function $u_l^{\text{int}}(r)$ is expanded over some finite basis involving N linearly independent functions φ_j as

$$u_l^{\text{int}}(r) = \sum_{j=1}^N c_j \varphi_j(r). \quad (3.4)$$

The functions φ_j must vanish at the origin but are not necessarily orthogonal. In contrast to some traditional presentations of the R -matrix theory [8], we do not assume that they satisfy specific boundary conditions at $r = a$. Various choices are possible, as exemplified in section 4. The internal and external pieces of the radial functions will be connected at the boundary a by the continuity of the wave function u_l and of its first derivative.

The R matrix at energy E is defined through⁴

$$u_l(a) = R_l(E)[au'_l(a) - Bu_l(a)]. \quad (3.5)$$

A dimensionless boundary parameter B is included for later convenience. Its choice will be discussed later. The inverse of the R matrix is thus the difference between the logarithmic derivative of the radial wave function at the boundary between both regions and the boundary parameter B . This matrix has dimension 1 in a single-channel case and is just a function of energy. In multichannel problems, the dimension of the R matrix is equal to the number of channels (see section 3.10). The principle of the method relies on the facts that the R matrix can be calculated from properties of the Hamiltonian in the internal region and that its knowledge allows determining the scattering matrix in the external region.

The operator H_l is not Hermitian over the internal region $(0, a)$. This property is not convenient for practical resolutions of the Schrödinger equation. This problem is elegantly solved with the help of the surface operator introduced by Bloch [11]

$$\mathcal{L}(B) = \frac{\hbar^2}{2\mu} \delta(r - a) \left(\frac{d}{dr} - \frac{B}{r} \right). \quad (3.6)$$

The operator $H_l + \mathcal{L}(B)$ is Hermitian over $(0, a)$ when B is real [11]. Moreover, it has a fully discrete spectrum as the self-adjoint problem is defined over a finite interval.

The Schrödinger equation in the internal region is approximated by the inhomogeneous Bloch–Schrödinger equation

$$(H_l + \mathcal{L}(B) - E)u_l^{\text{int}} = \mathcal{L}(B)u_l^{\text{ext}}, \quad (3.7)$$

where the external solution is used in the right-hand member. The mathematical problem is complemented with the continuity condition

$$u_l^{\text{int}}(a) = u_l^{\text{ext}}(a). \quad (3.8)$$

Until now, the approximation only consists of using in the right-hand side of (3.7) the asymptotic form (2.19) which is

⁴ As defined here, the R matrix is dimensionless. In some works, it has the dimension of a length and differs from the present definition by a factor a . Definition (3.21) of the reduced width amplitudes must then be modified accordingly.

known except for the value of the scattering matrix U_l . The main advantage of the R -matrix method is that an expansion in square-integrable functions can now be used in the internal region.

Because of the Dirac function in the Bloch operator, (3.7) and (3.8) are equivalent to the Schrödinger equation (3.1) restricted to the interval $(0, a)$ supplemented by the continuity condition at $r = a$ [11],

$$u_l^{\text{int}'}(a) = u_l^{\text{ext}'}(a) \quad (3.9)$$

for any B . Hence, beyond making $H_l + \mathcal{L}(B)$ Hermitian, the Bloch operator enforces the continuity of the derivative of the wave function. The importance of this aspect of the Bloch operator has often been underestimated in the literature. Condition (3.9) need not be imposed to the basis functions φ_j since the Bloch operator will impose it to the physical solution u_l . For historical reasons, a lot of confusion about the R matrix arose from the misunderstanding of this property as we shall see in section 3.5.

Formally, the inhomogeneous Bloch–Schrödinger equation (3.7) can be solved with the Green function defined by

$$(H_l + \mathcal{L}(B) - E)G_l(r, r') = \delta(r - r') \quad (3.10)$$

and $G_l(0, r) = 0$. The solution reads

$$u_l^{\text{int}}(r) = \int_0^a G_l(r, r') \mathcal{L}(B) u_l^{\text{ext}}(r') dr'. \quad (3.11)$$

With (3.6) and (3.5), the R matrix is thus given by

$$R_l(E) = \frac{\hbar^2}{2\mu a} G_l(a, a). \quad (3.12)$$

The calculable R -matrix method consists of solving the Bloch–Schrödinger equation with an approximate Green function expanded over a finite basis.

To obtain a practical expression for (3.12), expansion (3.4) is introduced in (3.7) and the resulting equation is projected on $\varphi_i(r)$, giving

$$\sum_{j=1}^N C_{ij}(E, B) c_j = \frac{\hbar^2}{2\mu a} \varphi_i(a) (a u_l^{\text{ext}'}(a) - B u_l^{\text{ext}}(a)). \quad (3.13)$$

The elements of the symmetric matrix C are defined as

$$C_{ij}(E, B) = \langle \varphi_i | T_l + \mathcal{L}(B) + V - E | \varphi_j \rangle. \quad (3.14)$$

Dirac brackets correspond here to one-dimensional integrals over the variable r from 0 to a . Because of the Bloch operator, the right-hand side of (3.13) only involves values at $r = a$.

Coefficients c_j are obtained by solving system (3.13). Introducing them in (3.4) at $r = a$ and comparing with (3.5) provides the calculable R matrix

$$R_l(E, B) = \frac{\hbar^2}{2\mu a} \sum_{i,j=1}^N \varphi_i(a) (C^{-1})_{ij} \varphi_j(a). \quad (3.15)$$

This expression is nothing but a finite-basis approximation of (3.12).

The wave function in the internal region is given by

$$u_l^{\text{int}}(r) = \frac{\hbar^2}{2\mu a R_l(E, B)} u_l^{\text{ext}}(a) \sum_{j=1}^N \varphi_j(r) \sum_{i=1}^N (C^{-1})_{ij} \varphi_i(a). \quad (3.16)$$

We shall see in section 3.4 that it does not depend on B .

3.3. Properties of the R matrix

Temporarily, in this section, the basis functions $\varphi_i(r)$ are assumed to be orthonormal. The matrix of overlaps $\langle \varphi_i | \varphi_j \rangle$ is thus the unit matrix. Let us consider the eigenvalues E_{nl} and the corresponding normalized eigenvectors v_{nl} of matrix $C(0, B)$,

$$C(0, B) v_{nl} = E_{nl} v_{nl} \quad (3.17)$$

with the orthonormality property

$$v_{nl}^T v_{n'l'} = \delta_{nn'}. \quad (3.18)$$

With the spectral decomposition

$$[C(E, B)]^{-1} = \sum_{n=1}^N \frac{v_{nl} v_{nl}^T}{E_{nl} - E}, \quad (3.19)$$

the R function (3.15) becomes

$$R_l(E, B) = \sum_{n=1}^N \frac{\gamma_{nl}^2}{E_{nl} - E} \quad (3.20)$$

with

$$\gamma_{nl} = \left(\frac{\hbar^2}{2\mu a} \right)^{1/2} \phi_{nl}(a) \quad (3.21)$$

and

$$\phi_{nl}(r) = \sum_{i=1}^N v_{nl,i} \varphi_i(r), \quad (3.22)$$

where $v_{nl,i}$ is the i th component of v_{nl} . The γ_{nl} are known as the reduced width amplitudes and their squares γ_{nl}^2 as the reduced widths [5]. Their interpretation is simple. They are proportional to the value at the channel radius of variational approximations ϕ_{nl} of the eigenfunctions of the Hermitian operator $H_l + \mathcal{L}(B)$. Those corresponding to the lowest energies thus represent approximate eigenfunctions of the physical problem confined over the interval $(0, a)$ with logarithmic derivative B at $r = a$.

Expression (3.20) looks familiar to practitioners of the R -matrix theory. It is however obtained here with a finite basis. The traditional expression for the R matrix is obtained when N tends towards infinity in a complete basis as

$$R_l(E, B) = \sum_{n=1}^{\infty} \frac{\gamma_{nl}^2}{E_{nl} - E}. \quad (3.23)$$

The energies E_{nl} are now the exact eigenvalues of the operator $H_l + \mathcal{L}(B)$ and the reduced width amplitudes γ_{nl} are related to the values at $r = a$ of its exact eigenfunctions.

The R matrix is a real function when V and B are real. It has an infinity of real simple poles, bounded from below. Its derivative is always positive at regular points. It is a meromorphic function of the energy when the energy is considered as a complex variable [5]. All residues are negative and given by minus the reduced widths γ_{nl}^2 .

3.4. Scattering matrix and phase shift

Since the R matrix is known, the external function (3.3) can be introduced in relation (3.8) to determine the scattering matrix for the l th partial wave as

$$U_l = e^{2i\phi_l} \frac{1 - (L_l^* - B)R_l(E, B)}{1 - (L_l - B)R_l(E, B)}. \quad (3.24)$$

In this expression,

$$L_l = ka \frac{O_l'(ka)}{O_l(ka)} \quad (3.25)$$

is the dimensionless logarithmic derivative of O_l at the channel radius, L_l^* is the conjugate of L_l , and

$$\phi_l = \arg I_l(ka) = -\arctan[F_l(ka)/G_l(ka)] \quad (3.26)$$

is the hard-sphere phase shift. Note that the same notation ϕ_l in [5] represents the opposite of the hard-sphere phase shift.

Expression (3.24) has the striking property that it does not depend on the boundary parameter B , independently of the size of the basis. Indeed, with the matrix relation (B4) in appendix B, one deduces from (3.15) and (3.14)

$$\frac{1}{R_l(E, 0)} = \frac{1}{R_l(E, B)} + B \quad (3.27)$$

for any B , real or complex. Expression (3.27) means that the logarithmic derivative of the internal wave function at the boundary is independent of B . Introducing relation (3.27) into (3.24) shows that any B value leads to the same scattering matrix as for $B = 0$. Equation (3.27) is well known in R -matrix theory (see equation (IV.2.5a) of [5]). It is also valid for the phenomenological R matrix with a finite number of poles [14]. However, its validity for the approximation (3.24) for any basis size [29, 57] is sometimes overlooked.

Like the scattering matrix U_l and the external wave function $u_l^{\text{ext}}(r)$, the internal function (3.16) does not depend on the choice for B . Indeed, with the help of relation (B3), one easily shows that, for any B , it is equal to the similar expression where B is replaced by zero.

For a better physical interpretation of the results which is important in applications, it is convenient to introduce some definitions. To this end, L_l is separated into its real and imaginary parts as

$$L_l = S_l + iP_l. \quad (3.28)$$

The real part S_l and imaginary part P_l of L_l are called the shift and penetration factors, respectively. They depend on energy and on the channel radius. The penetration factor can be written with the Wronskian relation $I_l O_l' - I_l' O_l = 2i$ as

$$P_l(E) = \frac{ka}{|O_l(ka)|^2} = \frac{ka}{F_l(ka)^2 + G_l(ka)^2}. \quad (3.29)$$

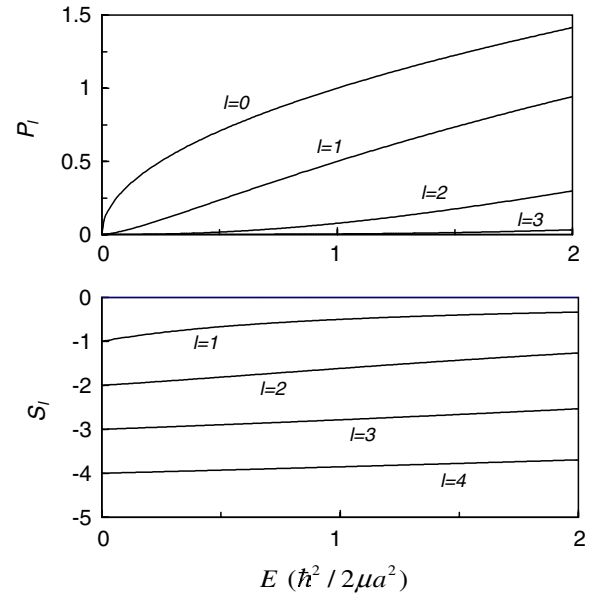


Figure 1. Penetration factors $P_l(E)$ (upper panel) and shift factors $S_l(E)$ (lower panel) in the neutral case ($\eta = 0$) as a function of E in units of $\hbar^2/2\mu a^2$.

It is always positive and increasing [5]. The shift factor reads

$$S_l(E) = P_l(E)[F_l(ka)F_l'(ka) + G_l(ka)G_l'(ka)]. \quad (3.30)$$

It is always negative for $\eta \geq 0$ [5]. Although we do not know a proof that S_l is always increasing in the same case, we could not find numerically a counterexample. As shown below, none of these properties is valid in the attractive case.

In the neutral case ($\eta = 0$), the penetration factors have simple analytical expressions such as

$$P_0(E) = ka, \quad P_l(E) = \frac{(ka)^3}{1 + (ka)^2}, \dots \quad (3.31)$$

They do not vary very fast with energy (see figure 1). This figure is universal, i.e. independent of the collision. Note that the derivative of P_0 with respect to energy is infinite at the origin. This property leads to the special behaviour of neutron scattering in the s wave. Penetration factors decrease with the orbital momentum l as expected from the occurrence of an increasing centrifugal barrier. The shift factors read

$$S_0(E) = 0, \quad S_l(E) = -\frac{1}{1 + (ka)^2}, \dots \quad (3.32)$$

They vary smoothly with energy, starting from the integer values $-l$ (see figure 1). This weak energy dependence is the origin of the Thomas approximation [5] where the shift factor is assumed to vary linearly in a limited energy range.

The penetration factors are very different according to whether both particles are charged or not. In the repulsive charged case, the energy dependence of the penetration factors is much stronger (note the logarithmic scale in figure 2). Here we have to choose the strength of the Coulomb interaction. Figure 2 corresponds to a channel radius a equal to the Bohr radius a_B . The strong dependence at low energies is due

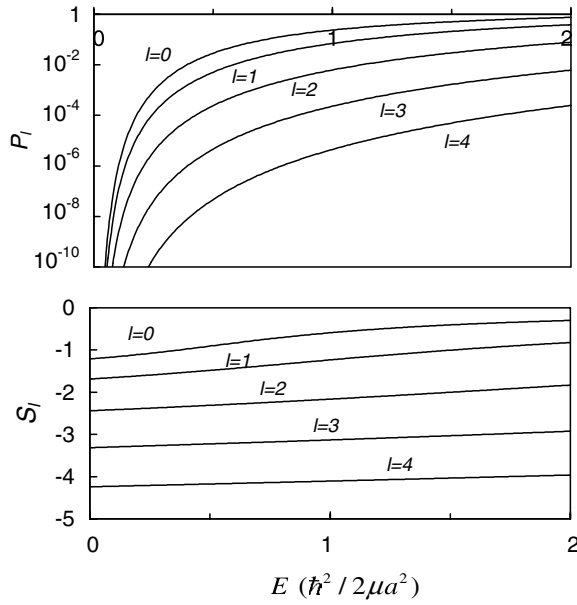


Figure 2. Penetration factors $P_l(E)$ (upper panel) and shift factors $S_l(E)$ (lower panel) in the repulsive charged case for $a = a_B$ as a function of E in units of $\hbar^2/2\mu a^2$.

to the difficulty of penetrating a Coulomb barrier when the scattering energy becomes much smaller than the height of this barrier. Beyond $l = 1$, increasing from l to $l + 1$ decreases the penetration factors by more than an order of magnitude. In contrast, shift factors are much more similar in all cases. In the repulsive charged case, the shift factors are quite similar to those of the neutral case, except for $l = 0$ (see figure 2).

In the attractive charged case, the energy dependence of the penetration factors is displayed in figure 3 for $a = a_B$. It is rather similar to the neutral case except at low energies where it starts from a finite value at energy zero. Shift factors displayed in figure 3 resemble other cases. Note, however, that S_0 is positive and decreasing.

With definition (3.28), the collision matrix (3.24) becomes

$$e^{2i\delta_l} = e^{2i\phi_l} \frac{1 - (S_l - B)R_l + iP_l R_l}{1 - (S_l - B)R_l - iP_l R_l}. \quad (3.33)$$

One obtains an explicit expression for the phase shift,

$$\delta_l = \phi_l + \arctan \frac{P_l R_l}{1 - (S_l - B)R_l}. \quad (3.34)$$

The internal wave function (3.16) can be rewritten as

$$u_l^{\text{int}}(r) = \frac{\hbar^2}{\mu a} e^{i(\delta_l - \frac{1}{2}\pi)} C_l \times \frac{(ka P_l)^{1/2}}{|1 - (L_l - B)R_l|} \sum_{j=1}^N \varphi_j(r) \sum_{i=1}^N (C^{-1})_{ij} \varphi_i(a), \quad (3.35)$$

which explicitly shows the phase and modulus of u_l^{int} (up to a global sign). For an orthonormal basis, this expression can be rewritten using (3.19) and (3.22) as

$$u_l^{\text{int}}(r) = \frac{\hbar^2}{\mu a} e^{i(\delta_l - \frac{1}{2}\pi)} C_l \frac{(ka P_l)^{1/2}}{|1 - (L_l - B)R_l|} \sum_{n=1}^N \frac{\phi_{nl}(r)\phi_{nl}(a)}{E_{nl} - E}. \quad (3.36)$$

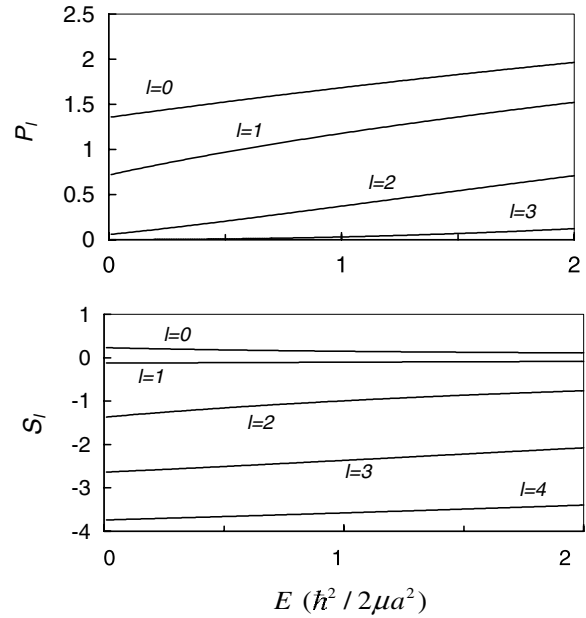


Figure 3. Penetration factors $P_l(E)$ (upper panel) and shift factors $S_l(E)$ (lower panel) in the attractive charged case for $a = a_B$ as a function of E in units of $\hbar^2/2\mu a^2$.

3.5. On the basis and boundary parameter choices

Considerable confusion exists in the literature about the properties that basis states φ_i should have. Improper choices have led to the introduction of corrections and to attempts to use the boundary parameter B to correct drawbacks of the basis. However, we have just seen that the results are independent of the choice of B . It is thus worthwhile to devote this section to a clarification of this issue that has sometimes led to an undeserved reputation of poor convergence for the calculable R -matrix method.

In their seminal paper, Wigner and Eisenbud wanted to provide a phenomenological description of resonances [3]. They did not intend to propose a technique of resolution. To reach their goal they assume that the basis functions all satisfy (for $B = 0$) the boundary conditions $\varphi_j(0) = 0$ and

$$a\varphi'_j(a) - B\varphi_j(a) = 0. \quad (3.37)$$

This procedure leads to the R matrix (3.23). When used as a technique of resolution, the finite-basis R matrix (3.15) or (3.20) obtained with this procedure does not converge uniformly. The reason is simple. The first derivative of the wave function (3.16) suffers from a discontinuity at $r = a$ [58]. The limit of $u_l^{\text{int}'}$ when r tends towards a to the left is equal to $u_l^{\text{ext}'}(a)$ but not to $u_l^{\text{int}'}(a)$,

$$\lim_{r \rightarrow a^-} u_l^{\text{int}'}(r) = u_l^{\text{ext}'}(a) \neq u_l^{\text{int}'}(a). \quad (3.38)$$

For example, if $B = 0$, $\varphi'_j(a)$ vanishes for all j values and one readily sees that $u_l^{\text{int}'}(a) = 0$ at all energies. This property has unfavourable consequences on the convergence of numerical methods when the basis is truncated since the logarithmic derivative of the external solution depends on the phase shift (and thus on energy) and cannot be matched with the internal

solution (see figures 5 and 8 in section 4). Buttle [27] has proposed a correction to the R -matrix truncation. His idea is to replace the truncated part by an analytical approximation, i.e., in practice, by the same expression for the zero potential. Although this correction improves the phase shifts, it does not really solve the problem because it does not improve the wave functions.

This problem received a solution with the works of Lane and Robson [28, 29, 59]. Their method was successfully applied in nuclear physics where traditional basis functions do not satisfy (3.37) and, on the contrary, display a variety of behaviours at the channel radius. With oscillator basis functions, accurate results for neutron–nucleus scattering could be obtained [59, 60]. At the same time, a microscopic extension of the R matrix using a fully antisymmetrized two-centre harmonic-oscillator model provided accurate phase shifts for collisions between light nuclei with few basis states [35, 36] (see section 6.2). The success of these calculations relies on the fact that the Bloch operator makes condition (3.37) unnecessary. Since the results do not depend on B , the choice $B = 0$ was used. A general although economical method for solving coupled-channel problems is described in [41].

The negative role of condition (3.37) remained long unnoticed in atomic physics where in many cases basis states were imposed to satisfy (3.37) [8, 51, 61–63]. In the literature, the basis functions are often assumed to be solutions of a Sturm–Liouville problem satisfying (3.37). As reviewed in [9], various solutions to the purported convergence problems of the calculable R matrix have been proposed, such as using two different sizes for the internal region. Another type of solution proposed in [64] requires a basis with a boundary condition depending on the eigenvalue E_{nl} . In 1983, Greene [65, 66] realized in the context of atomic physics that, in place of the traditional choice (3.37) of a common boundary condition to all basis functions at $r = a$, a variety of values for the logarithmic derivatives of the basis functions should be far more efficient for accurate calculations. He also proposed to optimize the boundary parameter B to have a better connection between the internal and external logarithmic derivatives. With his variational principle [66] applied to potential scattering, B is given at each energy E by the generalized eigenvalue problem

$$C(E, B)c = 0 \quad (3.39)$$

in the present notation. One readily sees [67] that the only eigenvalue B is $1/R(E)$ which, as the logarithmic derivative of the internal wave function, is obviously optimal. With this choice, the basis functions allow a perfect matching but at the cost of a new calculation of the basis at each energy. As we have shown with (3.27), this complication is unnecessary since all physical results are independent of B .

The first accurate calculations in atomic physics with a basis that fully ignores condition (3.37) can be found in [39, 68–70]. New developments making use of B splines now avoid this condition [71–73]. So let us emphasize that the calculable R matrix does converge accurately when the basis functions are a well chosen part of a complete set displaying a variety of logarithmic derivatives at the channel radius a . The reason for its accuracy is that the Bloch operator imposes

a good matching at the boundary [40]. The choice of a boundary parameter B is irrelevant and the Buttle correction is not necessary because the good matching of the internal and external wave functions allows an accurate determination of the phase shift. Practice has shown that this simple solution allows a much smoother connection with the external wave function [40, 41]. In opposition to the traditional presentation, there is thus no need for a special assumption about the behaviour of the basis functions at the boundary.

3.6. Resonances

Resonances can be studied in various ways. Each of them may be useful, either in calculable applications (section 4.8) or in phenomenological applications (section 5).

In a first approach, the boundary parameter can be chosen as [11, 29]

$$B = L_l. \quad (3.40)$$

It thus depends on energy. This complex value leads to a complex function $R_l(E, L_l)$ which is not an R matrix in the strict sense since B is not a real constant. It is the function introduced by Kapur and Peierls [4]. Nevertheless, it is also given by expression (3.15). Equation (3.24) then takes the simpler form [29, 46]

$$U_l = e^{2i\phi_l} [1 + (L_l - L_l^*)R_l(E, L_l)]. \quad (3.41)$$

This expression is also valid for complex k values if ϕ_l is defined as the phase of $I_l(ka)$. Since (3.41) has no denominator, a direct relation appears between a pole of the scattering matrix, i.e. a resonance energy, and a pole of the complex R matrix. This relation is, however, valid only when L_l is calculated at the resonance energy. This means that the scattering and R matrices have only one common pole and only at specific energies. Determining S -matrix poles in this way thus requires some iterative procedure. The choice (3.40) for the boundary parameter can be used to analyse the mathematical nature of resonances in the complex plane in coupled-channel cases [74]. However, the same results can also be interpreted with the traditional R matrix involving only real parameters [75]. Let us return to real energies for the other approaches. We choose $B = 0$ to simplify the presentation.

Another definition of a resonance energy E_R is that it corresponds to the value $\pi/2$ of the resonant part $\delta_l - \phi_l$ of the phase shift. From (3.34), it is therefore defined by the equation

$$1 - S_l(E_R)R_l(E_R) = 0. \quad (3.42)$$

In general, this equation must be solved numerically. To define the resonance width, let us consider the collision matrix (3.33) for energies close to E_R . A Taylor expansion of $S_l(E)R_l(E)$ for $E \approx E_R$ provides the Breit–Wigner approximation

$$U_l^{\text{BW}}(E) \approx e^{2i\phi_l} \frac{E_R - E + i\Gamma(E)/2}{E_R - E - i\Gamma(E)/2}. \quad (3.43)$$

In this expression the (energy-dependent) width of the resonance is given by

$$\Gamma(E) = \frac{2P_l(E)R_l(E)}{[d(S_l R_l)/dE]_{E=E_R}}. \quad (3.44)$$

Because of the shift of E_R with respect to a pole (see below), $R_l(E)$ can be supposed to vary slowly near a narrow resonance (see section 5). The total width then reads

$$\Gamma(E) = 2\gamma^2 P_l(E) = \frac{P_l(E)}{P_l(E_R)} \Gamma(E_R), \quad (3.45)$$

where $\Gamma(E_R)$ is the width at the resonance energy. The reduced width γ^2 defined by (3.45) is given by

$$\gamma^2 = R_l(E_R)/[d(S_l R_l)/dE]_{E=E_R}. \quad (3.46)$$

Let us mention that (3.42) may have solutions which do not correspond to physical states. The width of a physical resonance should be small enough to make its lifetime longer than the typical collision time.

In another way of studying a resonance, let us consider an energy very close to a pole E_{nl} of the R matrix. If all terms with $n' \neq n$ can be neglected, the R matrix is approximated as $R_l(E, 0) \approx \gamma_{nl}^2/(E_{nl} - E)$. A simple calculation provides

$$\delta_l \approx \phi_l + \arctan \frac{\gamma_{nl}^2 P_l(E)}{E_{nl} - \gamma_{nl}^2 S_l(E) - E}. \quad (3.47)$$

This expression resembles the Breit–Wigner form of the phase shift

$$\delta_l^{\text{BW}} \approx \phi_l + \arctan \frac{\frac{1}{2}\Gamma(E)}{E_R - E}. \quad (3.48)$$

By comparison, one defines the resonance energy

$$E_R = E_{nl} - \gamma_{nl}^2 S_l(E_R) \quad (3.49)$$

and the formal width

$$\Gamma(E) = 2\gamma_{nl}^2 P_l(E). \quad (3.50)$$

The resonance energy is defined by an implicit equation which can be solved approximately (see section 5.2). The width is an energy-dependent quantity whose asymmetric shape depends on the behaviour of P_l . Its relation with a measured width is also discussed in section 5.2.

With (3.21), (3.49) and (3.50), the internal wave function (3.36) can be approximated at the vicinity of a resonance by

$$u_l^{\text{int}}(r) \approx e^{i(\delta_l - \frac{1}{2}\pi)} C_l \left[\frac{\hbar v \Gamma}{(E_R - E)^2 + (\Gamma/2)^2} \right]^{1/2} \phi_{nl}(r). \quad (3.51)$$

It is thus proportional to an approximate eigenfunction (3.22) of $H_l + \mathcal{L}(0)$ with a proportionality factor exhibiting the usual Lorentzian energy dependence of a resonance. Equation (3.51) is at the basis of the so-called bound-state approximations where the resonance is described by a square-integrable wave function [76].

3.7. Bound states

The R -matrix formalism can be extended to bound states ($E_B < 0$) [37]. In that case the external wave function u_l^{ext} is given by

$$u_l^{\text{ext}}(r) = C_l W_l(2\kappa_B r), \quad (3.52)$$

where $W_l(x)$ is a shorthand notation for the Whittaker function (2.10) and where κ_B and η_B are the wave number and Sommerfeld parameter, respectively, of the bound state. In (3.52), C_l is the asymptotic normalization constant (ANC) which determines the amplitude of the wave function at large distances. This quantity plays an important role in some nuclear reactions of astrophysical interest [77] (see section 5.7).

To determine E_B , a convenient choice for the boundary parameter B in (3.6) is

$$B = L_l(E_B) = S_l(E_B) = 2\kappa_B a \frac{W'_l(2\kappa_B a)}{W_l(2\kappa_B a)}, \quad (3.53)$$

because it suppresses the right-hand side of the Bloch–Schrödinger equation (3.7). Since the wave function is real, L_l is real and identical to the shift factor. The penetration factor P_l vanishes. The internal wave function is expanded over a basis, as in (3.4). Projecting the Bloch–Schrödinger equation (3.7) over a basis function φ_i provides for $i = 1, N$,

$$\sum_{j=1}^N \langle \varphi_i | T_l + \mathcal{L}(L_l) + V - E_B | \varphi_j \rangle c_j = 0. \quad (3.54)$$

This system of equations is similar to a standard eigenvalue problem, but parameter L_l depends on energy E_B . In practice, one starts from $L_l = 0$ and iterates until energy E_B has converged. At convergence, the c_j can be calculated by solving the system. If u_l^{int} is normed according to (3.18), the square of the norm of the wave function is given by

$$N_l = 1 + (C_l)^2 \int_a^\infty (W_l(2\kappa_B r))^2 dr. \quad (3.55)$$

This expression can be rewritten [5, 17] as

$$N_l = 1 + \gamma_{nl}^2 \left[\frac{dS_l}{dE} \right]_{E=E_B}, \quad (3.56)$$

where γ_{nl} is the reduced width amplitude of the bound state.

The internal wave function is given by (3.16) multiplied by $N_l^{-1/2}$,

$$u_l^{\text{int}}(r) = N_l^{-1/2} \sum_{j=1}^N v_{nl,j} \varphi_j(r). \quad (3.57)$$

where coefficients $v_{nl,j}$ correspond for an orthogonal basis to the eigenvector v_{nl} of $C(0, L_l)$ at energy $E_{nl} = E_B$ in (3.17). Using (3.22), it can be rewritten as

$$u_l^{\text{int}}(r) = N_l^{-1/2} \phi_{nl}(r). \quad (3.58)$$

From (3.8) and (3.52), the ANC is given by

$$C_l = N_l^{-1/2} \phi_{nl}(a) / W_l(2\kappa_B a) \quad (3.59)$$

or with (3.21) by [78]

$$C_l = (2\mu a / \hbar^2 N_l)^{1/2} \gamma_{nl} / W_l(2\kappa_B a). \quad (3.60)$$

It should be independent of radius a . This relation between the ANC and a reduced width amplitude which corresponds to a vanishing width can be useful for the phenomenological R matrix. A similar formalism can be applied to resonances [79], and provides widths as well as energies of resonances.

3.8. Capture cross sections

The determination of capture cross sections requires the calculation of matrix elements of the electromagnetic multipole operators $\mathcal{M}_{\mu}^{\sigma\lambda}$ between an initial scattering state and a final bound state. One can take into account the division of the configuration space in the general case [37] but the principle of the calculation can be explained more easily in the simple potential model using equations (2.57), (2.58) and (2.64).

According to the R -matrix framework, the radial matrix element between an initial scattering wave function $u_i(r) \equiv u_{I_i l_i}(r)$ and a final bound-state wave function $u_f(r) \equiv u_{I_f l_f}(r)$ appearing in (2.64) can be written for an electric multipole as

$$\int_0^\infty u_f r^\lambda u_i dr = \int_0^a u_f^{\text{int}} r^\lambda u_i^{\text{int}} dr + \int_a^\infty u_f^{\text{ext}} r^\lambda u_i^{\text{ext}} dr. \quad (3.61)$$

The internal matrix element is given by

$$\int_0^a u_f^{\text{int}} r^\lambda u_i^{\text{int}} dr = \sum_{k,k'} c_{f,k'} c_{i,k} \int_0^a \varphi_{k'} r^\lambda \varphi_k dr, \quad (3.62)$$

where coefficients $c_{f,k'}$ and $c_{i,k}$ are related to the final and initial wave functions, respectively. Note that the bases could be different for both states. In the external region, we have

$$\begin{aligned} \int_a^\infty u_f^{\text{ext}} r^\lambda u_i^{\text{ext}} dr \\ = C_i C_f \int_a^\infty W_{l_i}(2\kappa_B r) r^\lambda (I_{l_i}(kr) - U_{I_i l_i}^J O_{l_i}(kr)) dr. \end{aligned} \quad (3.63)$$

As for elastic scattering, the total matrix element (3.61) should not depend on the channel radius a , whereas each contribution does depend on a . For transitions to weakly bound states, the external term is dominant since the Whittaker function slowly decreases at large distances. Neglecting completely the internal contribution leads to the ‘external-capture’ model [80]. A typical example is the ${}^7\text{Be}(p,\gamma){}^8\text{B}$ reaction where the ground state is bound by 137 keV only [77]. In contrast, resonant reactions or transitions to deeply bound states provide a dominant internal term.

3.9. Propagation methods

For long-range potentials, the channel radius may become very large. This may induce a prohibitive size for the R -matrix basis and lead to long computation times. This problem was first met in atomic physics because of the long tail of polarization potentials and led to the development of propagation methods [32, 81, 82]. This situation can also occur in nuclear physics, for example, in three-body systems [83] or in coupled-channel calculations [84].

Different methods have been proposed to address this problem. The basic idea is either to propagate the wave function or the R -matrix over several intervals on which the basis size remains reasonable or to determine ‘distorted’ Coulomb functions valid at distances shorter than the channel

radius. We present here a propagation method directly derived for the R -matrix (see for example [82]).

The idea of propagation methods [32] is to divide the internal region $(0, a)$ in N_s subregions $(a_{\alpha-1}, a_\alpha)$ for $\alpha = 1, N_s$, with $a_0 = 0$ and $a_{N_s} = a$. The intermediate radii a_α can be chosen equidistant, but this is not mandatory. The width of the intervals and the basis size in each interval can also depend on the number of oscillations of the wave function [81, 82]. With small intervals, the R -matrix bases remain limited, but the number N_s of repetitions of the calculation may be large. Approximations of the potential can often be employed in some intervals. In some cases, the size of the intervals is chosen small enough so that the potential may be considered as constant which allows an analytical propagation [32].

We briefly present here the principle of the propagation technique for potential scattering with a basis in each interval. We refer to references [81, 82] for a multichannel extension. A Bloch operator \mathcal{L}_α is now defined at each boundary a_α as

$$\mathcal{L}_\alpha = \frac{\hbar^2}{2\mu} \delta(r - a_\alpha) \frac{d}{dr}, \quad \alpha = 1, N_s. \quad (3.64)$$

The Bloch–Schrödinger equation is replaced by a set of equations

$$\begin{aligned} (H_l + \mathcal{L}_\alpha - \mathcal{L}_{\alpha-1} - E) u_{l,\alpha} &= (\mathcal{L}_\alpha - \mathcal{L}_{\alpha-1}) u_{l,\alpha}, \\ \alpha &= 1, N_s \end{aligned} \quad (3.65)$$

with $\mathcal{L}_0 = 0$. The boundary conditions are $u_{l,1}(0) = 0$ and

$$u_{l,\alpha}(a_\alpha) = u_{l,\alpha+1}(a_\alpha), \quad \alpha = 1, N_s \quad (3.66)$$

with $u_{l,N_s+1} \equiv u_l^{\text{ext}}$. In each interval, the wave function is expanded over a set of N_α basis functions

$$u_{l,\alpha}(r) = \sum_{j=1}^{N_\alpha} c_j^\alpha \varphi_j^\alpha(r). \quad (3.67)$$

Equation (3.65) can be solved with approximate Green functions as in section 3.2. By projecting (3.65) on one of the basis functions, the solutions can be approximated as

$$u_{l,\alpha}(r) = \sum_{jj'} (C_\alpha^{-1})_{jj'} \langle \varphi_{j'}^\alpha | \mathcal{L}_\alpha - \mathcal{L}_{\alpha-1} | u_{l,\alpha} \rangle \varphi_j^\alpha(r), \quad (3.68)$$

where the symmetric matrix C_α is defined in each interval by

$$C_{\alpha,ii'} = \langle \varphi_i^\alpha | H_l + \mathcal{L}_\alpha - \mathcal{L}_{\alpha-1} - E | \varphi_{i'}^\alpha \rangle. \quad (3.69)$$

The Dirac notation represents an integration limited to the range $(a_{\alpha-1}, a_\alpha)$.

For each interval, (3.68) can be used to determine a relation between values of the wave function and its first derivative at $a_{\alpha-1}$ and a_α ,

$$u_{l,\alpha}(a_{\alpha-1}) = \mathcal{R}_{10}^\alpha u'_{l,\alpha}(a_\alpha) - \mathcal{R}_{11}^\alpha u'_{l,\alpha}(a_{\alpha-1}), \quad (3.70)$$

$$u_{l,\alpha}(a_\alpha) = \mathcal{R}_{00}^\alpha u'_{l,\alpha}(a_\alpha) - \mathcal{R}_{01}^\alpha u'_{l,\alpha}(a_{\alpha-1}), \quad (3.71)$$

where various values of the approximate Green functions $\mathcal{R}_{\beta\beta'}^\alpha$ are defined as

$$\mathcal{R}_{\beta\beta'}^\alpha = \frac{\hbar^2}{2\mu} \sum_{jj'} \varphi_j^\alpha(a_{\alpha-\beta}) (C_\alpha^{-1})_{jj'} \varphi_{j'}^\alpha(a_{\alpha-\beta'}) \quad (3.72)$$

with $\beta\beta' = 0, 1$.

An R matrix can be defined at each boundary with an extension of (3.5) as

$$u_{l,\alpha}(a_\alpha) = a_\alpha R(a_\alpha) u'_{l,\alpha}(a_\alpha), \quad \alpha = 1, N_s. \quad (3.73)$$

Equations (3.70), (3.71) and (3.73) provide relationships between R matrices at $a_{\alpha-1}$ and a_α ($\alpha = 2, N_s$),

$$a_{\alpha-1} R(a_{\alpha-1}) = -\mathcal{R}_{11}^\alpha + \mathcal{R}_{10}^\alpha [\mathcal{R}_{00}^\alpha - a_\alpha R(a_\alpha)]^{-1} \mathcal{R}_{01}^\alpha, \quad (3.74)$$

$$a_\alpha R(a_\alpha) = \mathcal{R}_{00}^\alpha - \mathcal{R}_{01}^\alpha [\mathcal{R}_{11}^\alpha + a_{\alpha-1} R(a_{\alpha-1})]^{-1} \mathcal{R}_{10}^\alpha. \quad (3.75)$$

The latter equation provides an outwards propagation [$R(a_\alpha)$ from $R(a_{\alpha-1})$] and the former provides a backwards propagation [$R(a_{\alpha-1})$ from $R(a_\alpha)$]. This technique is quite efficient in multichannel calculations. Numerically the main part of the R -matrix calculation arises in the inversion of matrices C_α (see (3.72)). It may save computer time to diagonalize them when many energies are needed. The size of these matrices is given by the number of basis functions times the number of channels. If the calculation involves many channels, reducing the number of basis functions may lead to a significant reduction of the computer times.

The collision matrix is obtained from $R(a_{N_s})$ with (3.24). The external wave function u_l^{ext} is thus known. By starting from the last interval, the wave function is determined by its coefficients in each interval. If the $\mathcal{L}_{\alpha-1}$ terms are simplified in (3.65), one obtains the system

$$\sum_{j'} [C_{\alpha,jj'} + \langle \varphi_j^\alpha | \mathcal{L}_{\alpha-1} | \varphi_{j'}^\alpha \rangle] c_{j'}^\alpha = \langle \varphi_j^\alpha | \mathcal{L}_\alpha | u_{l,\alpha} \rangle \quad (3.76)$$

where (3.73) can be used to eliminate $u'_{l,\alpha}(a_\alpha)$ in the right-hand side. The matrix in this system can be inverted with (B2). Starting with $\alpha = N_s$ and going backwards one obtains the coefficients in all intervals.

Let us briefly discuss other techniques dealing with long-range potentials. In [83], in the framework of three-body continuum states, we propagate the wave functions from $a_{\alpha-1}$ to a_α by using the Numerov algorithm. This approach avoids the choice of a basis, but requires longer computer times. It is also difficult to apply to non-local potentials.

The Light-Walker propagation consists of approximating the potential by a constant in small enough intervals [32]. In [84], this method is improved by considering linear approximations of the potential. In the method suggested by Gailitis [85], the Coulomb wave functions are modified by $1/r$ expansions, which can be used at short distances (see also [82, 86]).

3.10. Extension to multichannel collisions

Until now the presentation was, for the sake of clarity and simplicity, limited to single-channel calculations which also neglect the spins of the colliding particles. This does not affect the general properties of the R -matrix theory. However, many problems require a multichannel approach.

In a many-body problem, the Schrödinger equation (2.33) involves Hamiltonian (2.25). The total wave function $\Psi^{JM\pi}$ of the system, with total angular momentum J and parity π , is expanded over a set of channel states (2.29), denoted as $|c\rangle$. If we assume that a single relative coordinate appears in the problem or that we approximate all relative coordinates by a single one, the wave function is given by (2.43). The Schrödinger equation is replaced by a set of differential equations

$$\sum_{c'} [(T_c + E_c - E) \delta_{cc'} + V_{cc'}] u_{c'} = 0, \quad (3.77)$$

where, as before, T_c includes the centrifugal term. This system is a particular case or a local approximation of (2.38).

A typical example is given by coupled-channel calculations where channel states are defined by (2.29). This situation occurs, for example, in coupled-channel calculations with a discretized continuum (CDCC) [87], see section 6.3. Another example corresponds to three-body scattering, where the channel states $|c\rangle$ contain various quantum numbers defined in the hyperspherical formalism [88], see section 6.4.

In all cases the problem is first to determine the potentials $V_{cc'}$ and then to solve (3.77) for positive energies. Here we essentially deal with the second step. We thus assume that the potentials are known and that they present the asymptotic behaviour

$$V_{cc'} \xrightarrow{r \rightarrow \infty} \frac{Z_{1c} Z_{2c} e^2}{r} \delta_{cc'}. \quad (3.78)$$

In these conditions the asymptotic form of the radial wave functions $u_c(r)$ is given by (2.34) and the radial wave functions in the external region at energy E are defined as

$$u_{c(c_0)}^{\text{ext}}(r) = \begin{cases} v_c^{-1/2} (I_c(k_c r) \delta_{cc_0} - U_{cc_0} O_c(k_c r)) & \text{for } E_c < E, \\ A_{cc_0} W_{-\eta_c, l+\frac{1}{2}}(2\kappa_c r) & \text{for } E_c > E, \end{cases} \quad (3.79)$$

where c_0 is the entrance channel ($E_{c_0} < E$).

The Bloch operator (3.6) is defined in the multichannel formalism as

$$\mathcal{L} = \sum_c |c\rangle \mathcal{L}_c \langle c|, \quad \mathcal{L}_c = \frac{\hbar^2}{2\mu_c} \delta(r-a) \left(\frac{d}{dr} - \frac{B_c}{r} \right), \quad (3.80)$$

where coefficients B_c are chosen as zero or as in (3.53) for open and closed channels, respectively. Note that these coefficients then depend on energy for closed channels. This choice may be inefficient in some variants of the R matrix [59] but is convenient in (3.88) and (3.89) below. The Bloch-Schrödinger equation is given by

$$\sum_{c'} [(T_c + \mathcal{L}_c + E_c - E) \delta_{cc'} + V_{cc'}] u_{c'}^{\text{int}} = \mathcal{L}_c u_c^{\text{ext}}. \quad (3.81)$$

The internal parts of the radial wave functions are expanded over a basis $\varphi_j(r)$,

$$u_c^{\text{int}}(r) = \sum_{j=1}^N c_{cj} \varphi_j(r). \quad (3.82)$$

The determination of the R matrix and of the collision matrix U are direct extensions of the formalism developed in sections 3.2 and 3.4.

The R matrix is defined from

$$u_c(a) = \sum_{c'} (\mu_c/\mu_{c'})^{1/2} R_{cc'} [a u_{c'}'(a) - B_{c'} u_{c'}(a)]. \quad (3.83)$$

Matrix R is symmetric, with elements given by

$$R_{cc'}(E) = \frac{\hbar^2}{2\sqrt{\mu_c \mu_{c'}} a} \sum_{i,i'=1}^N \varphi_i(a) (C^{-1})_{ci,c'i'} \varphi_{i'}(a), \quad (3.84)$$

where

$$C_{ci,c'i'} = \langle \varphi_i | T_c + \mathcal{L}_c + E_c - E | \varphi_{i'} \rangle \delta_{cc'} + \langle \varphi_i | V_{cc'} | \varphi_{i'} \rangle. \quad (3.85)$$

As in section 3.3, the spectral decomposition of the symmetric matrix C for an orthonormal basis provides the canonical form of the multichannel R matrix as

$$R_{cc'}(E) = \sum_n \frac{\gamma_{nc} \gamma_{nc'}}{E_n - E}, \quad (3.86)$$

where the real poles E_n are the eigenvalues of C and the reduced width amplitude of pole E_n in channel c is expressed as a function of the components of the corresponding normed eigenvector v_n as

$$\gamma_{nc} = \left(\frac{\hbar^2}{2\mu_c a} \right)^{1/2} \sum_{i=1}^N v_{n,ci} \varphi_i(a). \quad (3.87)$$

The number of terms in the sum (3.86) is given by the product of the number of channels by N .

The collision matrix is obtained with

$$U = Z^{-1} Z^*, \quad (3.88)$$

where an element of matrix Z reads

$$Z_{cc'} = (k_c a)^{-1/2} [O_c(k_c a) \delta_{cc'} - k_{c'} a R_{cc'} O_{c'}'(k_{c'} a)]. \quad (3.89)$$

For complex potentials as encountered in the optical model, expression (3.88) must be modified into

$$U = Z_O^{-1} Z_I, \quad (3.90)$$

where $Z_O = Z$ and $Z_I \neq Z_O^*$ is given by a similar expression with outgoing functions replaced by incoming ones. Matrix U is then not unitary.

The dimension of the R matrix is equal to the number of channels included in the calculation; it does not depend on energy. In contrast, the dimension of the collision matrix U is given by the number of *open* channels and may vary with energy. In (3.89), only open channels contribute thanks

to the choice of boundary parameters B_c . The R matrix can be modified by eliminating the closed channels. When not all channels are open, let us denote open channels by c and closed channels by \bar{c} . Equation (3.84) remains valid with matrix C replaced by a smaller open-channel matrix C^o with elements [5, 41, 89]

$$C_{ci,c'i'}^o = C_{ci,c'i'} - \sum_{\bar{c}j,\bar{c}'j'} \langle \varphi_i | V_{c\bar{c}} | \varphi_j \rangle (\bar{C}^{-1})_{\bar{c}j,\bar{c}'j'} \langle \varphi_{j'} | V_{\bar{c}'c'} | \varphi_{i'} \rangle, \quad (3.91)$$

where \bar{C} is the restriction of the full matrix to closed channels and \bar{c}, \bar{c}' are the corresponding indices.

The internal components of the wave function are given for both open and closed channels by

$$u_{c(c_0)}^{\text{int}}(r) = \sum_{c'} \frac{\hbar^2 k_{c'}}{2\mu_{c'} v_{c'}^{1/2}} [I_{c'}'(k_{c'} a) \delta_{c'c_0} - U_{c'c_0} O_{c'}'(k_{c'} a)] \times \sum_{i,i'=1}^N \varphi_i(r) (C^{-1})_{ci,c'i'} \varphi_{i'}(a), \quad (3.92)$$

where the sum over c' runs over open channels only. The coefficients of the external part of the wave function for closed channels read

$$A_{\bar{c}c_0} = [W_{-\eta_{\bar{c}},l+\frac{1}{2}}(2\kappa_{\bar{c}} a)]^{-1} \times \sum_{c'} (\mu_c k_{c'}/\hbar)^{1/2} a R_{\bar{c}c'} [I_{c'}'(k_{c'} a) \delta_{c'c_0} - U_{c'c_0} O_{c'}'(k_{c'} a)], \quad (3.93)$$

where the sum over c' also runs over open channels only.

4. Applications of the calculable R matrix

4.1. Conditions of the calculations

In this section we apply the calculable R -matrix method to the scattering by a potential. Our goal is not to fit experimental data, but to illustrate the method under different conditions, and with different types of basis functions. In this approach, both colliding particles are assumed to be structureless, and to interact through a potential (see (3.2)). In general, this potential $V(r)$ involves a local term $U(r)$ and a non-local term $W(r, r')$ such that

$$V(r) u_l(r) = U(r) u_l(r) + \int_0^\infty W(r, r') u_l(r') dr'. \quad (4.1)$$

In the following, unless specified otherwise, only the local term is included. In nuclear physics applications, the local potential $U(r)$ usually contains a nuclear and a Coulomb contributions, denoted as $V_N(r)$ and $V_C(r)$, respectively. The potential may be l dependent, by adapting its parameters to the l value. The Schrödinger equation associated with potential (4.1) can be solved exactly (at the computer precision) with the Numerov method [90–92]. The exact phase shifts and wave functions will be compared with the R -matrix calculations.

In nuclear-physics applications, the reduced mass is expressed in terms of the nucleon mass as

$$\mu = \frac{A_1 A_2}{A_1 + A_2} m_N, \quad (4.2)$$

where A_1 and A_2 are the nucleon numbers. The calculations are performed with $\hbar^2/2m_N = 20.736 \text{ MeV fm}^2$ and $e^2 = 1.44 \text{ MeV fm}$.

To cover a broad variety of applications, we have first selected three typical systems:

- (i) The $^{12}\text{C} + \text{p}$ system ($l = 0$) which presents a narrow resonance ($\Gamma = 37 \text{ keV}$) at $E = 0.42 \text{ MeV}$.
- (ii) The $\alpha + \alpha$ system ($l = 4$) which presents a broad resonance ($\Gamma = 3.5 \text{ MeV}$) near $E = 11.3 \text{ MeV}$.
- (iii) The $\alpha + {}^3\text{He}$ system ($l = 0$) which is non-resonant.

These cases are typical examples of nuclear-physics applications, and will be treated by different types of basis functions. Here, we only consider real potentials. This is consistent with the low-energy regime where the R -matrix method is well adapted. The extension to complex potentials is, however, trivial.

Then, the calculation of $e^- - \text{H}$ phase shifts will provide a typical example of an atomic-physics application with a non-local potential. Atomic units will be used.

4.2. Basis functions

We consider different families of basis functions $\varphi_i(r)$ ($i = 1, \dots, N$, see (3.4)) vanishing at $r = 0$, commonly used in the literature. The corresponding matrix elements are given in [appendix C](#).

- (i) *Sine functions*. The basis functions are given by

$$\varphi_i(r) = \sin \frac{\pi r}{a} (i - 1/2). \quad (4.3)$$

This choice seems natural since it can simulate the oscillating behaviour of the wave function near the channel radius. However, we will show that these basis functions are not suitable for accurate calculations since the derivative satisfies (3.37) (see section 3.5), i.e. it vanishes at $r = a$ for each i value,

$$\varphi'_i(a) = 0. \quad (4.4)$$

This property means that any finite combination of these basis functions will present a zero derivative at $r = a$. As discussed before, the matching between the internal and external solutions is therefore expected to be poor, and the R -matrix phase shifts rather inaccurate.

- (ii) *Gaussian functions*. The basis functions have a Gaussian dependence [43] with different size parameters

$$\varphi_i(r) = r^{l+1} \exp(-(r/b_i)^2), \quad (4.5)$$

where the b_i are chosen as a geometric progression

$$b_i = b_1 x_0^{i-1}, \quad (4.6)$$

and are therefore determined by a set of two parameters (b_1, x_0). Gaussian-type basis functions (4.5) allow an analytical calculation of the overlap and kinetic-energy matrix elements. For Gaussian potentials, the matrix elements are analytical as well.

- (iii) *Lagrange functions*. The Lagrange functions [42] are defined in the $(0, a)$ interval as

$$\varphi_i(r) = (-1)^{N+i} \left(\frac{r}{ax_i} \right)^n \sqrt{ax_i(1-x_i)} \frac{P_N(2r/a-1)}{r-ax_i}, \quad (4.7)$$

where P_N is the Legendre polynomial of order N , and x_i are the zeros of

$$P_N(2x_i-1) = 0. \quad (4.8)$$

In (4.7), the factor $(r/ax_i)^n$ is aimed at regularizing the basis function at the origin. For two-body calculations defined in the $(0, a)$ range, we use $n = 1$, which ensures that the wave function vanishes at the origin.

The basis functions satisfy the Lagrange conditions

$$\varphi_i(ax_j) = (a\lambda_i)^{-1/2} \delta_{ij}, \quad (4.9)$$

where λ_i is the weight of the Gauss–Legendre quadrature corresponding to the $(0, 1)$ interval. This basis is exactly equivalent to the Legendre basis defined by

$$\varphi_i(r) = r P_{i-1}(2r/a-1). \quad (4.10)$$

However, if the matrix elements with basis functions (4.7) are computed at the Gauss approximation of order N , consistent with the N mesh points, their calculation is strongly simplified. At this approximation, the overlap is given by

$$\langle \varphi_i | \varphi_j \rangle = \int_0^a \varphi_i(r) \varphi_j(r) dr \approx \delta_{ij}, \quad (4.11)$$

and the local-potential matrix is diagonal with elements just given by the value of the potential at the mesh points,

$$\langle \varphi_i | U | \varphi_j \rangle = \int_0^a \varphi_i(r) U(r) \varphi_j(r) dr \approx U(ax_i) \delta_{ij}. \quad (4.12)$$

This calculation is easily extended to non-local potentials $W(r, r')$

$$\langle \varphi_i | W | \varphi_j \rangle \approx a \sqrt{\lambda_i \lambda_j} W(ax_i, ax_j). \quad (4.13)$$

These matrix elements do not need any evaluation of integral. The kinetic-energy term is given by analytical expressions [93] (see [appendix C](#)). This method has been shown to be quite efficient and accurate in various fields for bound states [93] as well as for scattering states [42, 83]. In the present applications, the Gauss approximation will be used systematically, except in the $e^- - \text{H}$ scattering, where this approximation will be also tested by a Simpson quadrature for the matrix elements.

4.3. Application to a narrow resonance: $^{12}\text{C} + \text{p}$

The $^{12}\text{C} + \text{p}$ system is known to present a narrow resonance ($J^\pi = 1/2^+$, $E_R = 0.42 \text{ MeV}$, $\Gamma = 37 \text{ keV}$ [94]) at low energies. As mentioned before, our aim is not to fit these properties accurately, but to compare the exact solutions of the

Schrödinger equation (3.1) with the R -matrix approach. For the nuclear and Coulomb potentials we choose

$$V_N(r) = -73.8 \exp(-(r/2.70)^2),$$

$$V_C(r) = 6e^2/r. \quad (4.14)$$

In what follows, the units in the nuclear potentials are fm and MeV for lengths and energies, respectively. This potential reproduces the resonant behaviour of the s phase shifts at 0.42 MeV. To simulate the Pauli principle, a nucleus–nucleus potential may contain additional (unphysical) bound states [95, 96]. These Pauli forbidden states show up in microscopic calculations, where the internal structure of the colliding nuclei is taken into account, but their effect can be partly simulated in non-microscopic theories by additional bound states in the potential (see [95, 96] for details). For the $^{12}\text{C} + \text{p}$ system, the $l = 0$ potential contains one forbidden state.

In figure 4, we present the exact phase shifts and R -matrix calculations with Lagrange (a) and Sine (b) functions. The channel radius is chosen as $a = 8$ fm, where the nuclear interaction is negligible. Figure 4(a) shows that with the Lagrange functions, the convergence is reached with $N \geq 10$. We show an example with $N = 7$, where N is aimed at being not large enough. Figure 4(b) illustrates the Sine functions, poorly adapted to a good matching since the left derivative of the wave function at $r = a$ is zero (see (4.4)). Even $N = 20$ is far from the exact calculation. In figure 4(c), we present the convergence as a function of the channel radius with the Lagrange functions ($N = 15$ is fixed). Results obtained with Gaussian functions (with $b_1 = 1.4$ fm, $x_0 = 0.6$) are identical at the scale of the figure. As expected, $a = 5$ fm is too small ($|V_N(a)/V_C(a)| = 1.4$). To obtain a good stability, radii larger than 6 fm should be used.

The matching problem is illustrated in figure 5, where we show the wave function at $E = 2$ MeV, with $a = 8$ fm, $N = 15$. With the Lagrange functions, the matching between internal and external wave functions is quite smooth. For Sine functions, the matching is poor, which has a direct impact on the phase shifts.

The accuracy of the different basis functions is illustrated in table 1 where we compare various calculations of the phase shifts. The relative difference between left and right derivatives provides the matching parameter ϵ defined as

$$\epsilon = \frac{|u_l^{\text{ext}'}(a) - u_l^{\text{int}'}(a)|}{[u_l^{\text{ext}'}(a) + u_l^{\text{int}'}(a)]/2}. \quad (4.15)$$

This comparison is done for the different bases and at four typical energies. When ϵ is small, the matching is obviously accurate. However, in some specific cases where $u_l^{\text{ext}'}(a) + u_l^{\text{int}'}(a)$ is small, this parameter may be large, although the phase shift is fairly good. This parameter should therefore be considered as indicative only. Table 1 confirms that Lagrange and Gaussian functions represent a convenient basis, whereas Sine functions do not provide satisfactory results. Note that the use of Gaussian functions implies two additional parameters (b_1, x_0) to define the basis. This choice has to be optimized for the different conditions and is therefore less direct than Lagrange functions.

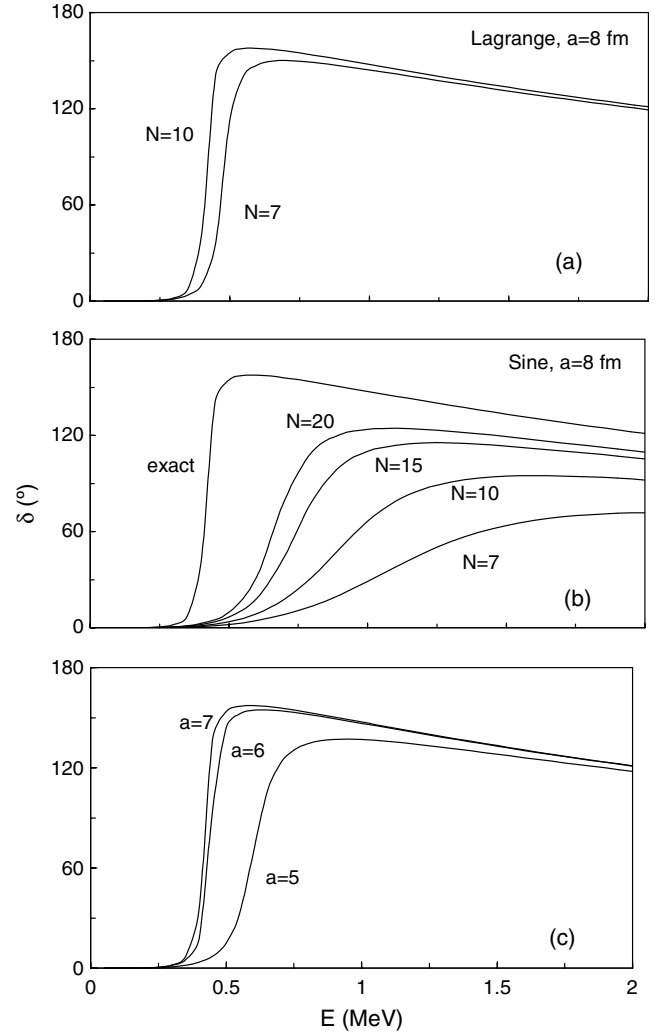


Figure 4. $^{12}\text{C} + \text{p}$ R -matrix phase shifts (in degrees) for different bases and conditions ($l = 0$). (a) Lagrange functions at $a = 8$ fm (the exact results are superimposed to the $N = 10$ curve), (b) Sine functions at $a = 8$ fm, (c) convergence as a function of a for $N = 15$; the Lagrange and Gaussian results are superimposed ($a = 7$ fm corresponds to the exact results).

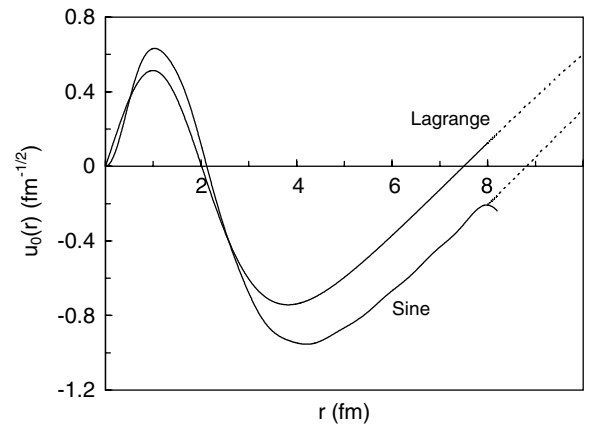


Figure 5. $^{12}\text{C} + \text{p}$ $l = 0$ wave functions with Lagrange and Sine functions at $E = 2$ MeV ($a = 8$ fm, $N = 15$). Solid lines represent the internal wave function and dotted lines the external parts. The Lagrange wave function is superimposed to the exact result.

Table 1. $^{12}\text{C} + p$ $l = 0$ phase shifts (in degrees) and matching parameters (4.15) for different bases ($a = 8$ fm).

E (MeV)	Phase shift				Matching parameter		
	Exact	$N = 7$	$N = 10$	$N = 15$	$N = 7$	$N = 10$	$N = 15$
<i>Lagrange</i>							
0.5	154.66	112.90	154.94	154.59	5.96	0.65	0.01
1.0	147.48	144.22	147.55	147.48	3.68	0.28	0.00
1.5	133.30	311.02	133.35	133.30	1.67	0.20	0.00
2.0	121.18	299.30	121.23	121.18	1.21	0.16	0.00
<i>Gaussian</i>							
0.5	154.66	179.36	154.53	154.53	5.61	0.02	0.01
1.0	147.48	146.52	147.47	147.47	0.04	0.01	0.01
1.5	133.30	130.28	133.29	133.29	1.06	0.00	0.01
2.0	121.18	112.15	121.18	121.18	1.55	0.01	0.01
<i>Sine</i>							
0.5	154.66	2.03	3.74	6.68	0.12	0.66	1.54
1.0	147.48	28.90	66.57	109.98	1.30	4.66	29.35
1.5	133.30	63.84	94.53	113.28	11.46	6.97	3.53
2.0	121.18	71.76	92.24	105.34	5.73	3.14	2.38

4.4. Application to a broad resonance: $\alpha + \alpha$

The $\alpha + \alpha$ system presents a well-known rotational band based on the 0^+ ground state. The $l = 0$ narrow resonance corresponds to the unstable ground state of ^8Be . In order to illustrate the R -matrix formalism applied to a broad resonance, we consider the $l = 4$ partial wave. The experimental energy and width of the resonance are $E_R = 11.35 \pm 0.15$ MeV and $\Gamma \approx 3.5$ MeV [97]. However, for broad resonances these properties may depend on the definition used (see section 3.6). A comparison between experiment and theory cannot be done with a high precision.

The $\alpha + \alpha$ potential of Buck *et al* [98] has a simple Gaussian form, is l -independent, and reproduces the $l = 0, 2, 4$ experimental $\alpha + \alpha$ phase shifts up to about 20 MeV. It is defined by

$$V_N(r) = -122.6225 \exp(-(r/2.132)^2),$$

$$V_C(r) = 4e^2 \text{erf}(r/1.33)/r. \quad (4.16)$$

Figure 6 shows the phase shifts obtained with the Lagrange and Sine functions, with $a = 8$ fm. With Lagrange functions, the R -matrix perfectly reproduces the exact phase shifts with $N \geq 10$. With Sine functions, the convergence is, as expected, much slower. Table 2 gives the phase shifts and ϵ values under different conditions and at different energies. Again, the importance of the matching on the phase shifts is obvious.

4.5. Application to a non-resonant system: $\alpha + ^3\text{He}$

For $l = 0$, the experimental $\alpha + ^3\text{He}$ phase shifts are well reproduced by the potential of Buck and Merchant [99],

$$V_N(r) = -66.10 \exp(-(r/2.52)^2),$$

$$V_C(r) = 4e^2(3 - (r/r_C)^2)/2r_C \text{ for } r \leq r_C, \\ = 4e^2/r \text{ for } r \geq r_C, \quad (4.17)$$

with $r_C = 3.095$ fm. In figure 7, we use the Lagrange functions for two radii: $a = 8$ fm, and $a = 5$ fm. For $a = 8$ fm, the convergence is reached as soon as $N \geq 10$. In contrast, the

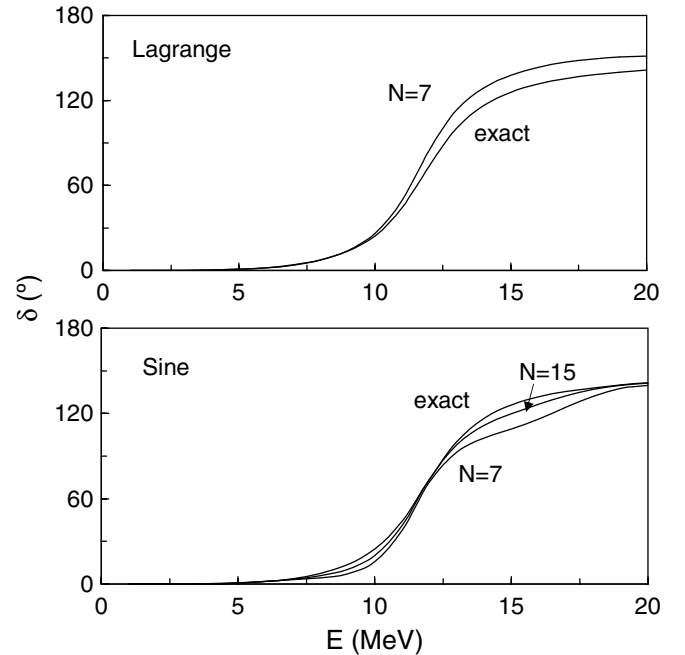


Figure 6. $\alpha + \alpha$ $l = 4$ phase shifts with the Lagrange and Sine functions for different N values. For the Lagrange functions $N \geq 10$ is indistinguishable from the exact result.

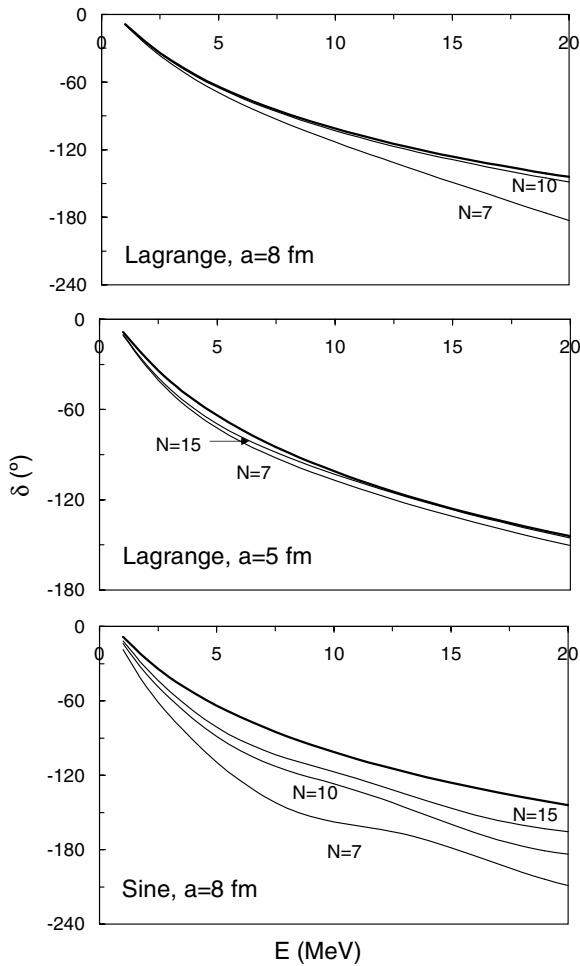
choice $a = 5$ fm is not consistent with one of the R -matrix requirements: the nuclear contribution is not negligible. In that case, it is impossible to get a good convergence at all energies.

In figure 8, we compare the wave functions at $E = 8$ MeV with the Sine and Lagrange functions. In the former case, the matching between the internal and external wave functions is poor, which has an impact on the accuracy of the phase shifts. Conversely, the R -matrix wave function with the Lagrange basis is indistinguishable from the exact wave function.

Table 3 gives the phase shifts and matching coefficients under different conditions. For $a = 8$ fm, a Lagrange basis with $N \geq 10$ provides reasonable phase shifts. If a increases (we choose here $a = 10$ fm), the R -matrix approximation is of course still valid, but the number of basis functions must be

Table 2. $\alpha + \alpha$ $l = 4$ phase shifts (in degrees) and matching parameters for Lagrange and Sine bases ($a = 8$ fm).

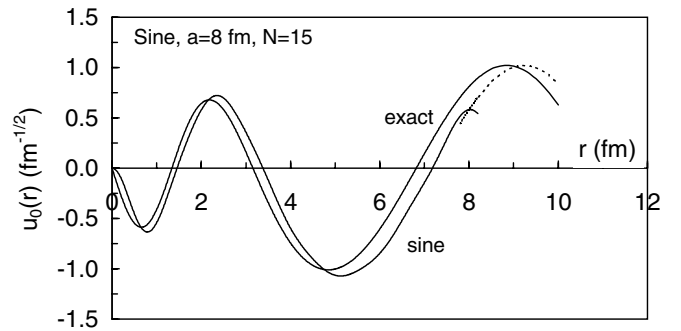
E (MeV)	Phase shift				Matching parameter		
	Exact	$N = 7$	$N = 10$	$N = 15$	$N = 7$	$N = 10$	$N = 15$
<i>Lagrange</i>							
5	0.79	0.81	0.80	0.80	0.05	0.02	0.00
10	24.46	26.19	24.58	24.48	0.42	0.12	0.00
15	125.88	137.90	126.00	125.88	0.31	0.18	0.01
20	141.55	151.24	141.53	141.54	1.26	5.67	0.13
<i>Sine</i>							
5	0.79	0.53	0.62	0.68	0.66	0.65	0.65
10	24.46	15.55	17.74	19.84	2.23	2.20	2.17
15	125.88	109.09	116.76	119.87	2.16	2.09	2.06
20	141.55	139.82	141.24	141.37	3.27	5.84	6.21

**Figure 7.** $\alpha + {}^3\text{He}$ R -matrix phase shifts with Lagrange ($a = 8$ fm and $a = 5$ fm) and Sine ($a = 8$ fm) functions for $l = 0$. The thick lines represent the exact phase shifts.

increased. This is expected as the internal wave function must be reproduced in a wider range. In agreement with figure 8, the Sine functions provide a poor approximation of the phase shifts.

4.6. Application to a deep potential

As mentioned before, the potential may contain additional (unphysical) bound states to simulate the Pauli principle. In the applications considered so far, the potentials involved a small

**Figure 8.** $\alpha + {}^3\text{He}$ $l = 0$ wave functions with Sine functions at $E = 8$ MeV ($a = 8$ fm, $N = 15$). Solid lines represent the internal wave function and the dotted line the external part with Sine functions. The Lagrange wave function is superimposed to the exact result.

number of forbidden states. The situation is different in heavy-ion reactions, where the number m_l of forbidden states may be rather large. In such conditions the internal wave function presents several oscillations which must be reproduced by the basis functions to provide accurate phase shifts.

This problem is illustrated here with the ${}^{13}\text{C} + {}^{12}\text{C}$ system ($l = 0$, $m_l = 12$). We take the deep Gaussian potential of [100] (depth of -273.7 MeV and range of 3.06 fm) for the nuclear interaction. The Coulomb potential has a point-sphere shape (see (4.17)), with a radius of 8.2 fm. The R -matrix phase shifts are determined with the Lagrange basis, and compared in figure 9 (upper panel) with the exact phase shifts. The channel radius is $a = 10$ fm. It is clear that small N values do not reproduce the phase shifts. Values larger than $N \approx 35$ are necessary to obtain accurate results.

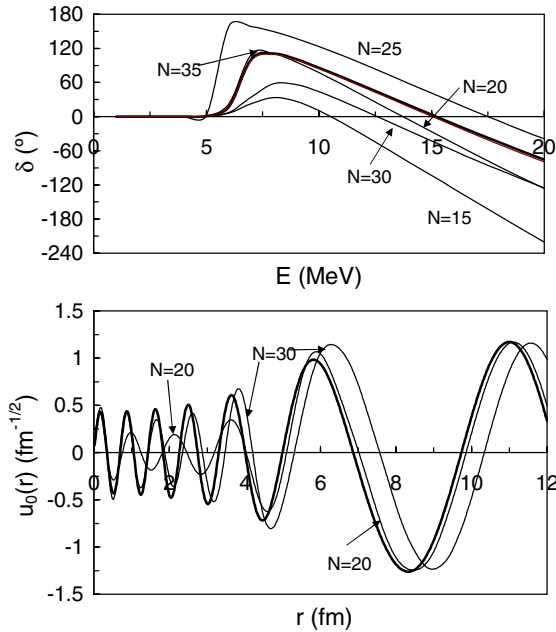
We show in figure 9 (lower panel) the wave function for $N = 20, 30, 40$ at $E = 10$ MeV. Clearly, $N = 20$ is not able to give a good description of the oscillations of the internal wave function. The situation is of course improved with $N = 30$, but only $N = 40$ is superimposed to the exact wave function. This problem is common to all potentials presenting many bound states.

4.7. Application to a non-local potential: $e^- - \text{H}$ scattering in the static-exchange approximation

The electron + hydrogen-atom scattering has been studied with various methods [51]. In the simplest version, referred to as

Table 3. $\alpha + {}^3\text{He}$ $l = 0$ phase shifts (in degrees) and matching parameters for different bases.

E (MeV)	Phase shift			Matching parameter	
	Exact	$N = 10$	$N = 15$	$N = 10$	$N = 15$
<i>Lagrange, $a = 8$ fm</i>					
5	-63.97	-65.02	-63.96	0.16	0.01
10	-101.2	-103.1	-101.2	0.89	0.22
15	-125.9	-128.9	-125.9	0.13	0.01
20	-144.2	-148.5	-144.2	0.14	0.02
<i>Lagrange, $a = 10$ fm</i>					
5	-63.97	-70.25	-63.97	0.30	0.04
10	-101.2	-109.5	-101.3	0.17	0.02
15	-125.9	-134.5	-126.0	5.19	0.07
20	-144.2	-149.4	-144.3	0.28	0.02
<i>Sine, $a = 8$ fm</i>					
5	-63.97	-88.74	-81.18	2.66	2.47
10	-101.2	-127.0	-117.2	1.16	0.81
15	-125.9	-159.4	-146.5	2.66	2.40
20	-144.2	-183.7	-165.4	1.95	1.82

**Figure 9.** Upper panel: ${}^{13}\text{C} + {}^{12}\text{C}$ $l = 0$ phase shifts with the Lagrange functions ($a = 10$ fm). Lower panel: corresponding wave functions at $E = 10$ MeV. The exact wave function (superimposed on the $N = 40$ result) is shown as a thick line.

(This figure is in colour only in the electronic version)

the static-exchange approximation [101, 102], the problem is limited to a single-channel calculation, but involves a non-local potential. The local term $U(r)$ reads

$$U(r) = -E_0 \left(\frac{a_0}{r} + 1 \right) \exp(-2r/a_0). \quad (4.18)$$

We use here the traditional atomic units, involving the Bohr radius a_0 and the Hartree energy $E_0 = e^2/a_0$

The non-local contribution is defined as

$$W(r, r') = (-1)^{S+1} \frac{4r r'}{a_0^3} \times \exp\left(-\frac{r+r'}{a_0}\right) \left(E - E_0 \left(1 + \frac{a_0}{r_{>}}\right)\right), \quad (4.19)$$

where E is the total energy, S is the total spin of the electrons ($S = 0$ or 1) and $r_{>} = \max(r, r')$. The $1/r_{>}$ singularity is responsible for numerical problems [103], and deserves special attention in the literature.

This example is used to illustrate the applicability of the Lagrange functions for non-local potentials (note that the singlet phase shifts have been already determined in the R -matrix framework [51]). Here the Gauss approximation associated with the Lagrange basis is expected to present convergence problems, owing to the singularity mentioned above. This problem will be addressed by performing, in parallel with the consistent Gauss approximation of the potential matrix elements (see (4.12) and (4.13)), a ‘traditional’ calculation using the Simpson method (with typically 1000 integration points) for the numerical quadrature.

Results are shown in tables 4 and 5 for $S = 0$ and $S = 1$, respectively, as a function of the wave number k . For the Lagrange-mesh method, we select a channel radius $a = 14 a_0$, and consider various basis sizes. Comparing with the alternative method (Simpson integration) which is less sensitive to singularities in the potential, we immediately see that a reasonable accuracy (typically 0.02 rad) can be achieved with small N values at the Gauss approximation. However, when N increases the convergence is rather slow. If we do not use the Gauss approximation for the potential matrix elements, at least five digits are exact with $N = 20$ and for a given a value. The sensitivity with respect to the channel radius is about 10^{-4} rad when going from $a = 14 a_0$ to $a = 16 a_0$. For comparison we give in table 4 the results of Burke *et al* [51], obtained for $S = 0$, up to $k = 0.7 a_0^{-1}$.

Similar conclusions can be drawn for the $S = 1$ phase shifts, but the Gauss approximation is slightly more accurate because the antisymmetry of the spatial part of the wave function decreases the effect of the $1/r_{>}$ singularity. The $S = 0$ and $S = 1$ phase shifts are also in good agreement with those of Apagyi *et al* [103] who use the Schwinger variational method [104], much more sensitive to numerical problems than the R -matrix method.

Table 4. R -matrix phase shifts (in rad.) for e^- -H scattering ($S = 0$). The potential matrix elements are computed, either with the associated Gauss approximation (4.12) and (4.13) or with the Simpson quadrature. The results are compared with those of Burke *et al* [51].

k (a_0^{-1})	Gauss approximation, $a = 14 a_0$					$N = 20$, Simpson		[51]
	$N = 20$	$N = 40$	$N = 60$	$N = 80$	$N = 100$	$a = 14 a_0$	$a = 16 a_0$	
0.1	2.3790	2.3917	2.3940	2.3949	2.3952	2.3959	2.3958	2.3960
0.2	1.8509	1.8654	1.8681	1.8691	1.8695	1.8703	1.8702	1.8704
0.3	1.4902	1.5036	1.5061	1.5070	1.5074	1.5081	1.5081	1.5081
0.4	1.2228	1.2352	1.2375	1.2384	1.2388	1.2394	1.2395	1.2391
0.5	1.0155	1.0274	1.0296	1.0304	1.0308	1.0314	1.0315	1.0309
0.6	0.8532	0.8650	0.8673	0.8681	0.8684	0.8691	0.8690	0.8685
0.7	0.7281	0.7401	0.7424	0.7432	0.7435	0.7442	0.7441	0.7438
0.8	0.6347	0.6470	0.6494	0.6502	0.6506	0.6513	0.6512	
0.9	0.5685	0.5813	0.5837	0.5846	0.5850	0.5857	0.5857	
1.0	0.5251	0.5384	0.5409	0.5417	0.5422	0.5429	0.5429	

Table 5. See caption to table 4 for $S = 1$.

k (a_0^{-1})	Gauss approximation, $a = 14 a_0$					$N = 20$, Simpson	
	$N = 20$	$N = 40$	$N = 60$	$N = 80$	$N = 100$	$a = 14 a_0$	$a = 16 a_0$
0.1	2.9080	2.9077	2.9077	2.9077	2.9077	2.9075	2.9076
0.2	2.6799	2.6794	2.6793	2.6792	2.6792	2.6791	2.6792
0.3	2.4622	2.4614	2.4612	2.4612	2.4611	2.4611	2.4611
0.4	2.2588	2.2576	2.2574	2.2574	2.2573	2.2572	2.2573
0.5	2.0721	2.0706	2.0703	2.0702	2.0702	2.0701	2.0701
0.6	1.9032	1.9013	1.9009	1.9008	1.9007	1.9006	1.9006
0.7	1.7521	1.7497	1.7492	1.7490	1.7490	1.7488	1.7488
0.8	1.6180	1.6150	1.6145	1.6143	1.6142	1.6140	1.6141
0.9	1.4998	1.4963	1.4957	1.4954	1.4953	1.4951	1.4952
1.0	1.3959	1.3919	1.3911	1.3909	1.3908	1.3905	1.3905

4.8. Discussion of resonances

In this section we determine the resonance energies and widths of the $^{12}\text{C} + \text{p}$ ($l = 0$) and $\alpha + \alpha$ ($l = 4$) systems, as an illustration of section 3.6. In figure 10, we show the functions $R(E)$ and $1/S(E)$ for both systems. The resonances energies are calculated from the roots of equation (3.42), i.e. from the crossing points of both curves. The numerical values, as well as the widths (3.45) are given in table 6.

The $^{12}\text{C} + \text{p}$ ($l = 0$) state is a typical example of a narrow resonance. The phase shifts near 0.42 MeV are well described by the Breit–Wigner approximation. Although the R matrices are rather different for $a = 8$ fm and $a = 10$ fm (see figure 10), the energy and width are weakly sensitive to the channel radius (see table 6). This result is typical of narrow and isolated resonances.

The situation is different for the $\alpha + \alpha$ ($l = 4$) system, which is typical of a broad resonance (around 12.5 MeV, see figure 6). The resonance properties are rather sensitive to the channel radius, whereas the phase shifts are almost identical. Table 6 shows that the second eigenvalue might be related to the 4^+ resonance. However, the width is not significantly smaller than the energy difference with neighbouring states. In that case, a single-level approximation is not well adapted to reproduce the phase shifts in a wide energy range.

4.9. Application to bound states

The R matrix is applied to the ^{13}N ground state ($J^\pi = 1/2^-, l = 1$) described by a $^{12}\text{C} + \text{p}$ potential model. In order to simulate the experimental binding energy (-1.94 MeV), the depth of the Gaussian potential used in section 4.3 for $l = 0$ has been modified to -55.3 MeV.

The calculation is performed with the Lagrange basis, and the results are presented in table 7. With $a = 8$ fm, $N = 7$ does not provide the exact energy. This situation is of course improved by increasing N . For $N = 15$, we have five exact digits, and the matching parameter is close to 0. In each case, four iterations are sufficient in system (3.54) to provide an energy stable by better than 0.1 keV. The ANC value C_l (see (3.52)) is also very stable.

As in section 4.3 for the phase shifts, the choice $a = 5$ fm is too small to make the nuclear interaction negligible. Although the matching parameter is quite acceptable, the convergence is slower and the final result does not converge to the exact energy. This means that a small matching parameter is not sufficient to ensure that the calculation is accurate. Testing the stability against the channel radius is a more severe test.

4.10. Application to a multichannel problem: $\alpha + d$

Here we use the $\alpha + \text{deuteron}$ potential of Dubovichenko [105] to investigate the R -matrix formalism in a multichannel

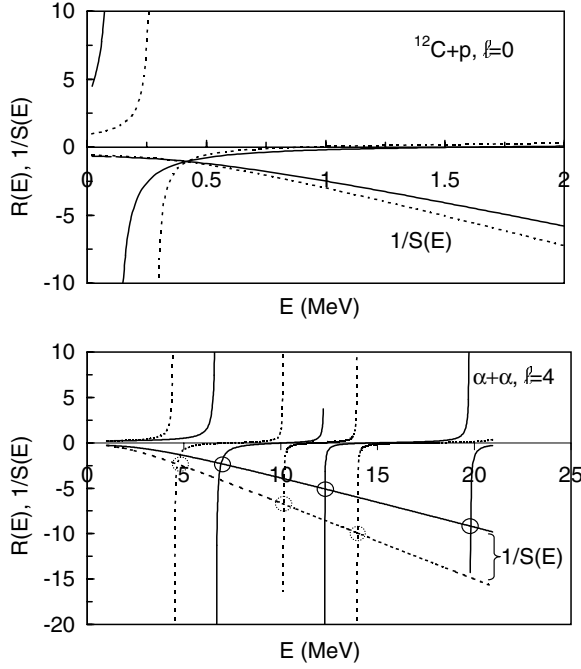


Figure 10. R -matrix $R_l(E)$ and inverse of the shift function $S_l(E)$ for the $^{12}\text{C} + \text{p}$ ($l = 0$) and $\alpha + \alpha$ ($l = 4$) collisions. Solid lines correspond to $a = 8$ fm and dotted lines to $a = 10$ fm. The circles show the roots of (3.42).

Table 6. Resonance energies and widths (in MeV) of the $^{12}\text{C} + \text{p}$ ($l = 0$) and $\alpha + \alpha$ ($l = 4$) systems. The Lagrange basis is used with $N = 15$.

Eigenvalue	$a = 8$ fm		$a = 10$ fm	
	E_R	$\Gamma(E_R)$	E_R	$\Gamma(E_R)$
$^{12}\text{C} + \text{p}$ ($l = 0$)				
1	0.418	0.0375	0.417	0.0369
$\alpha + \alpha$ ($l = 4$)				
1	6.92	5.14	4.67	3.68
2	12.3	2.47	10.2	2.74
3	19.8	7.08	14.0	3.33

problem. This nuclear potential $V_N(r)$ contains central $V_c(r)$ and tensor $V_t(r)$ forces, defined as

$$V_N(r) = V_c(r) + V_t(r)S_{12},$$

$$V_c(r) = V_0 \exp(-\alpha r^2),$$

$$V_t(r) = V_1 \exp(-\beta r^2), \quad (4.20)$$

where

$$S_{12} = \frac{6}{r^2} (\mathbf{S} \cdot \mathbf{r})^2 - 2S^2 \quad (4.21)$$

is the usual tensor operator. The Coulomb potential is the bare potential. With $V_0 = -91.979$ MeV, $V_1 = -25.0$ MeV, $\alpha = 0.2 \text{ fm}^{-2}$, $\beta = 1.12 \text{ fm}^{-2}$, this potential reproduces most of the ^6Li ground-state properties, in particular the binding energy, the quadrupole moment and the d-wave admixture amplitude. The spin and parity of the deuteron being 1^+ , non-natural parity states (i.e. $\pi = (-1)^{J+1}$) involve two l values:

Table 7. Energy of ^{13}N ground state (in MeV) with a Lagrange basis and different a and N values. The exact binding energy and ANC are -1.942 MeV and $2.063 \text{ fm}^{-1/2}$, respectively.

Iteration	$a = 8$, $N = 7$	$a = 8$, $N = 10$	$a = 8$, $N = 15$	$a = 5$, $N = 10$
1	-2.012	-2.052	-2.053	-3.236
2	-1.897	-1.940	-1.941	-1.763
3	-1.899	-1.941	-1.942	-1.894
4	-1.899	-1.941	-1.942	-1.881
5	-1.899	-1.941	-1.942	-1.882
6				-1.882
C_l ($\text{fm}^{-1/2}$)	2.060	2.071	2.072	2.034
ϵ	9.1	0.19	0.005	0.002

$l = |J - 1|$ and $l = J + 1$. The system to be solved (3.77) involves the potentials (we use the notation of section 3.10)

$$V_{11} = V_c + V_C - 2(J - 1)V_t/(2J + 1),$$

$$V_{12} = V_{21} = 6\sqrt{J(J + 1)}V_t/(2J + 1),$$

$$V_{22} = V_c + V_C - 2(J + 2)V_t/(2J + 1). \quad (4.22)$$

As in previous sections the R -matrix collision matrices are computed in various conditions, and compared with the ‘exact’ results obtained by the Numerov algorithm. The R -matrix calculations are performed with Lagrange functions. To compare with experiment [106], the collision matrix is diagonalized (see (2.37)) and parametrized as

$$U = \begin{pmatrix} \cos \epsilon & -\sin \epsilon \\ \sin \epsilon & \cos \epsilon \end{pmatrix} \begin{pmatrix} \exp(2i\delta_1) & 0 \\ 0 & \exp(2i\delta_2) \end{pmatrix} \times \begin{pmatrix} \cos \epsilon & \sin \epsilon \\ -\sin \epsilon & \cos \epsilon \end{pmatrix}, \quad (4.23)$$

where δ_1 and δ_2 are the (real) eigenphases and ϵ is the mixing angle (removing the tensor force provides $\epsilon = 0$). These values are presented in figure 11 for $J^\pi = 1^+$ and compared with the exact solutions (also shown in figures 4 and 5 of [105]). We choose $a = 8$ fm and show the result for $N = 7$. With this small number of basis functions, slight deviations can be observed. As soon as $N > 7$, the R -matrix phase shifts cannot be distinguished from the exact values.

Other applications of the R -matrix theory to multichannel problems can be found in [41].

4.11. Application to propagation methods

To illustrate the propagation of the R matrix, we present here a numerical example, with the $\alpha + \alpha$ system. We choose $a = 80$ fm, which is of course unnecessarily large for this system, but typical of long range potentials, where propagation methods should be used. The goal of this example is just to provide a numerical illustration of the method. The R matrix at 80 fm has been computed in three ways: (i) exactly with the Numerov algorithm, (ii) with 100 basis functions without propagation ($N_S = 1$), (iii) with 100 basis functions split into several equal intervals. The R -matrix basis functions are the

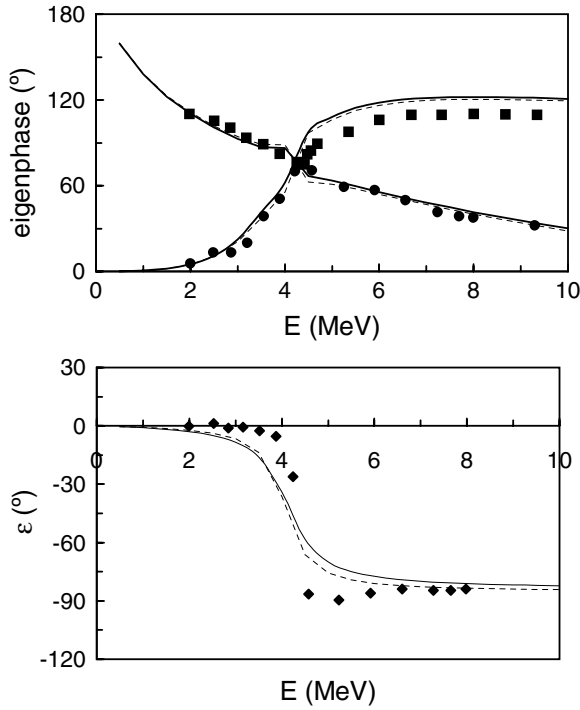


Figure 11. $\alpha + d$ eigenphases (upper panel) and mixing angles (lower panel) for $J^\pi = 1^+$. The solid lines represent the exact calculation and the dotted lines correspond to the R -matrix calculation with $a = 8$ fm, $N = 7$. The experimental data are taken from [106].

Lagrange functions. Matrix elements over an interval (a_1, a_2) are given in appendix C [see (C14)–(C18)].

Table 8 gives the $l = 0$ R -matrix at $a = 80$ fm for typical energies. Without propagation ($N_S = 1$), we reproduce at least four significant digits. This is still true for $N_S = 2$, but the computer time is reduced by more than a factor of two. Essentially the difference is that in the former case we have to invert one 100×100 matrix, whereas the latter calculation requires two inversions of 50×50 matrices. The computer time is still reduced with $N_S = 4$ (four inversions of 25×25 matrices). The precision is, however, reduced since the first interval (0.20 fm) only contains 25 basis functions. Increasing this number to 35 (and hence the full basis size to 110 functions) provides the exact R -matrix (with at least four significant digits) with similar computer times.

4.12. Application to capture reactions: $^{12}\text{C}(p,\gamma)^{13}\text{N}$

The $^{12}\text{C}(p,\gamma)^{13}\text{N}$ reaction is the first reaction of the CNO cycle. It represents an ideal candidate for an R -matrix treatment since the $1/2^+$ ($l = 0$) resonance at $E_R = 0.42$ MeV determines the S -factor (2.55) in a wide energy range. As in previous sections, our goal here is not to find the best fit to the data (see [17]). Rather, we want to illustrate the different contributions to the capture matrix elements (3.61), and to discuss various approximations. Our procedure is as follows:

- (i) The initial states are determined as in section 4.3.
- (ii) As our goal is to illustrate the different contributions to the capture matrix elements, the bound-state wave function

(and the corresponding ANC) is computed exactly with the Numerov algorithm [90]. This avoids the optimization of the basis for the bound state.

- (iii) The basis functions for the initial state are chosen as Lagrange functions ($N = 15$), and we determine the internal and external contributions from (3.62) and (3.63), respectively.

The matrix elements are computed as in section 3.8, but the R -matrix expansion of the final state is replaced by the exact wave function. Table 9 gives, at typical energies, the exact values of the matrix elements (i.e. with scattering wave functions obtained from the Numerov method), as well as their values in the R -matrix theory with $a = 8$ fm and $a = 10$ fm. Large values must be used to ensure that the nuclear interaction is negligible. Several comments can be made:

- (i) As expected the matrix element presents a maximum at $E = 0.42$ MeV, as the initial potential has been fitted to provide a resonance at this energy.
- (ii) Since the external scattering wave function (3.63) involves the phase shift, the external contribution also presents a resonant behaviour.
- (iii) Each term in (3.61) depends on the channel radius. Their sum, however, should be insensitive to its choice, if the conditions of the calculation are properly defined. The relative difference is maximum near the resonance but is always less than 1%.

For the sake of completeness we show in figure 12 the $^{12}\text{C}(p,\gamma)^{13}\text{N}$ S -factor compared with the available data sets [107, 108]. As usual in the potential model, a spectroscopic factor S should be introduced for a more realistic comparison with the data. The spectroscopic factor scales the total cross section. Values lower than unity mean that the final ground state is more complicated than a simple $^{12}\text{C} + p$ structure. With $S = 1$ the theoretical S -factor is larger than the data. A reasonable agreement can be obtained with $S = 0.45$, although the high energy part is slightly overestimated by the model.

5. The phenomenological R matrix

5.1. Introduction

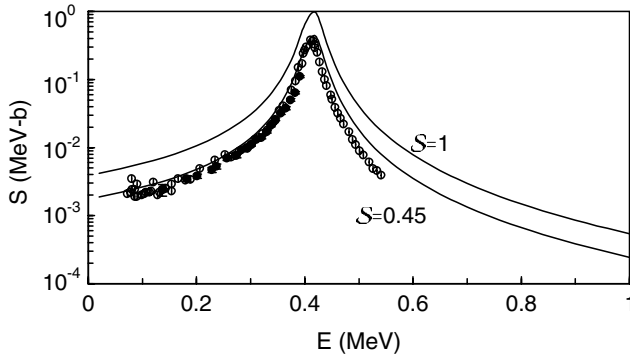
The goal of the phenomenological R -matrix method is to use a parametrization based on expression (3.20) of the R matrix or its multichannel generalization (3.86) with a finite number of poles. The properties of these poles are adjusted to some data, in place of being derived from some Hamiltonian, as in the calculable approach. We present here various applications in nuclear physics. In particular, this technique is very successful in nuclear astrophysics [109], where the main issue is to fit cross section data, and to extrapolate them down to stellar energies at which direct measurements are in general impossible (see, for example, [21]). Another recent application is the analysis of low-energy scattering data in experiments involving radioactive beams. Those experiments usually probe the nuclear structure at low level density, well adapted to the R -matrix formalism (see, for example references [110–112] for $^8\text{B} + p$, $^{10}\text{C} + p$ and $^{18}\text{Ne} + p$, respectively). The method is

Table 8. R -matrix for the $\alpha + \alpha$ collision ($l = 0$) and for different N_S values ($N = 100$, $a = 80$ fm). For each interval of size a/N_S the number of basis functions is $100/N_S$.

E (MeV)	Exact	$N_S = 1$	$N_S = 2$	$N_S = 4$
5	2.648×10^{-2}	2.648×10^{-2}	2.648×10^{-2}	2.643×10^{-2}
10	-3.729×10^{-1}	-3.729×10^{-1}	-3.730×10^{-1}	-3.957×10^{-1}
15	1.195×10^{-3}	1.195×10^{-3}	1.195×10^{-3}	1.157×10^{-3}
20	-1.246×10^{-2}	-1.246×10^{-2}	-1.246×10^{-2}	-1.262×10^{-2}
Time (ms)		1.2	0.50	0.25

Table 9. $^{12}\text{C}(p,\gamma)^{13}\text{N}$ matrix elements (see (3.62) and (3.63)) with Lagrange functions ($N = 15$).

E (MeV)	Exact			R -matrix		
	Internal	External	Total	Internal	External	Total
$a = 8$ fm						
0.20	220.78	76.56	297.34	219.24	76.51	295.74
0.40	2034.4	414.38	2448.8	2002.1	410.58	2412.7
0.60	247.93	19.26	267.18	246.76	19.32	266.08
0.80	116.02	-3.83	112.19	115.35	-3.81	111.54
1.00	74.60	-9.69	64.92	74.14	-9.68	64.46
$a = 10$ fm						
0.20	248.93	48.41	297.34	247.97	48.42	296.40
0.40	2240.6	208.22	2448.8	2228.7	208.03	2436.7
0.60	266.55	0.63	267.18	265.39	0.64	266.03
0.80	121.69	-9.49	112.19	121.13	-9.49	111.64
1.00	76.28	-11.37	64.92	75.92	-11.36	64.56

**Figure 12.** $^{12}\text{C}(p,\gamma)^{13}\text{N}$ S -factors with different spectroscopic factors S . The experimental data are from [107] (open circles) and [108] (closed circles).

of course not limited to elastic scattering, but can be extended to inelastic [113] as well as to transfer [114] reactions.

One of the main drawbacks of the phenomenological R -matrix formalism is that, although the pole energies and reduced widths are associated with physical properties, they cannot be directly compared with experiment. In particular, the R -matrix parameters significantly depend on the channel radius. This is in contrast to the so-called ‘observed’ data, such as resonance energies and widths directly fitted to experimental data which are by definition independent of such a radius. However, these ‘observed’ values of the energy and width of a resonance depend on the assumptions made about the theoretical description of the resonance (see section 3.6 for a part of the possible definitions). Within the phenomenological R -matrix approach, the ‘observed’ quantities have a rather

precise definition from which the R -matrix parameters can be determined. For an isolated resonance in some partial wave l , the observed energy E_R and width Γ_R are obtained in the single-channel approach by fitting the elastic cross section (2.46) where the phase shift is parametrized by the generalized Breit–Wigner expression (3.48),

$$\delta_l^{\text{BW}} \approx \phi_l + \arctan \frac{\frac{1}{2}\Gamma_R}{E_R - E}. \quad (5.1)$$

This expression may be simplified by neglecting ϕ_l or made more realistic by multiplying Γ_R by $P_l(E)/P_l(E_R)$. Note that, except for the simplest Breit–Wigner approximation, these expressions slightly depend on a through ϕ_l or P_l . The ‘observed’ reduced width γ_{obs}^2 is then extracted from Γ_R with the relation similar to (3.50),

$$\Gamma_R = 2\gamma_{\text{obs}}^2 P_l(E_R). \quad (5.2)$$

The corresponding ‘formal’ parameters, i.e. the pole location E_{nl} and the reduced width γ_{nl}^2 can then be deduced for a given channel radius a but their determination is not immediate because of the shift factor S_l and its energy dependence. The problem is more complicated if several resonances or several channels must be taken into account.

In the next sections, we present different methods to link the ‘formal’ R -matrix parameters with the ‘observed’ values. The simplest and most common case deals with a single isolated resonance, described by one pole (section 5.2). However, some applications require including several poles in the same partial wave or, in other words, considering interference effects between these poles (section 5.3). Other

applications require taking several channels into account (section 5.4). As a first application, we consider the $^{12}\text{C} + \text{p}$ elastic scattering from 0.3 to 1.8 MeV, where accurate data have existed for many years (section 5.5). Then a more recent multichannel application to $^1\text{H}(^{18}\text{Ne}, \text{p})^{18}\text{Ne}(\text{g.s.})$ and $^1\text{H}(^{18}\text{Ne}, \text{p}')^{18}\text{Ne}^*(2^+, 1.887 \text{ MeV})$ will be shown as an example of radioactive-beam experiments (section 5.6). Finally, the R -matrix method will be applied to radiative-capture reactions, with $^{12}\text{C}(\text{p}, \gamma)^{13}\text{N}$ as a typical example (section 5.7).

5.2. Single-pole approximation of elastic scattering

In section 3.6, we have presented a general procedure to define the resonance energy and width from the R -matrix expression. Let us particularize (3.23) to a single pole with energy E_1 and reduced width γ_1^2 (we drop the index l for the sake of clarity); the R matrix is then given by

$$R_l(E) = \frac{\gamma_1^2}{E_1 - E}. \quad (5.3)$$

This approximation is frequently used at low energy, where single isolated resonances are present. The R -matrix phase shift associated with (5.3) is given by (3.47). To go further, let us use the Thomas approximation [5], which consists of a linearization of the shift function $S_l(E)$. Near the pole energy E_1 , it reads

$$S_l(E) \approx S_l(E_1) + (E - E_1)S'_l(E_1), \quad (5.4)$$

where S'_l is the derivative of the shift factor with respect to energy (which appears both in the wave number k and in the Sommerfeld parameter η). The validity of this approximation is supported by figures 1, 2 and 3, where it is clear that, in a limited energy range, the linearization of the shift function is quite appropriate.

Comparing expression (3.47) of the phase shift at the Thomas approximation with the Breit–Wigner expression (5.1), one derives the observed properties (E_R, γ_{obs}) from the formal parameters (E_1, γ_1) of an isolated pole. The observed energy E_R reads

$$E_R = E_1 - \gamma_1^2 \frac{S_l(E_1)}{1 + \gamma_1^2 S'_l(E_1)}, \quad (5.5)$$

where the shift between both energies depends on E_1 . This shift also depends on a . It is in general non-negligible, unless γ_1^2 is very small. The observed reduced width reads

$$\gamma_{\text{obs}}^2 = \frac{\gamma_1^2}{1 + \gamma_1^2 S'_l(E_1)}. \quad (5.6)$$

It also depends on E_1 .

In practice, however, the reversed relationships are needed. Indeed, in many cases, observed values (E_R, γ_{obs}) are known from experiments (or from other theoretical works) and one wants to derive the corresponding R -matrix parameters (E_1, γ_1). The inverses of (5.5) and (5.6) are obtained by

Table 10. R -matrix parameters (5.7) and (5.8) for resonances in $^{12}\text{C} + \text{p}$ and $^{12}\text{C} + \alpha$ (in MeV). The observed reduced widths are obtained from (5.2).

	$a = 4 \text{ fm}$	$a = 5 \text{ fm}$	$a = 6 \text{ fm}$	$a = 7 \text{ fm}$
$^{12}\text{C} + \text{p} (J^\pi = 1/2^+, l = 0, E_R = 0.42 \text{ MeV}, \Gamma_R = 32 \text{ keV})$				
γ_{obs}^2	1.089	0.592	0.353	0.227
θ_{obs}^2	0.258	0.220	0.189	0.165
γ_1^2	3.083	1.157	0.569	0.323
E_1	-2.152	-0.614	-0.110	0.113
$^{12}\text{C} + \alpha (J^\pi = 1^-, l = 1, E_R = 2.42 \text{ MeV}, \Gamma_R = 420 \text{ keV})$				
γ_{obs}^2		0.574	0.277	0.165
θ_{obs}^2		0.6920	0.481	0.389
γ_1^2		1.172	0.374	0.191
E_1		0.491	1.921	2.219

linearizing the shift factor $S_l(E)$ around E_R as

$$\gamma_1^2 = \frac{\gamma_{\text{obs}}^2}{1 - \gamma_{\text{obs}}^2 S'_l(E_R)}, \quad (5.7)$$

$$E_1 = E_R + \gamma_1^2 S_l(E_R). \quad (5.8)$$

These results are well known [5].

In the literature, the reduced width is frequently expressed in units of the Wigner limit [89]

$$\gamma_W^2 = \frac{3\hbar^2}{2\mu a^2}, \quad (5.9)$$

which provides the dimensionless reduced widths

$$\begin{aligned} \theta_{\text{obs}}^2 &= \gamma_{\text{obs}}^2 / \gamma_W^2, \\ \theta_1^2 &= \gamma_1^2 / \gamma_W^2. \end{aligned} \quad (5.10)$$

Note that Lane and Thomas [5] define the dimensionless reduced width as $\theta^2 = \gamma_{\text{obs}}^2 \mu a^2 / \hbar^2$ without an explicit reference to the Wigner limit. In general, a value of θ^2 not far from unity indicates the occurrence of a cluster structure, i.e. the colliding nuclei partly conserve their identity within the resonance. Conversely, a plausible guess on θ^2 (possibly inspired by a model) can be used to estimate the width of a resonance. This concept of dimensionless reduced width, as defined by (5.10), was first used by various authors [115–117] in the interpretation of low-energy scattering data.

The difference between observed and formal parameters is illustrated by numerical applications in table 10 for the narrow $1/2^+$ resonance in $^{12}\text{C} + \text{p}$ ($E_R = 0.42 \text{ MeV}$, $\Gamma_R = 32 \text{ keV}$) and for the broad 1^- resonance in $^{12}\text{C} + \alpha$ ($E_R = 2.42 \text{ MeV}$, $\Gamma_R = 420 \text{ keV}$). The formal parameters (E_1, γ_1) are calculated for various channel radii and are then used to determine the phase shifts shown in figure 13. As usual in applications of the phenomenological R -matrix method, the channel radii are somewhat smaller than in the ‘calculable’ variant.

From table 10, it is clear that the dimensionless reduced widths θ_{obs}^2 are less dependent on the channel radius than γ_{obs}^2 . For both systems, and in particular for $^{12}\text{C} + \alpha$, the θ_{obs}^2 values are rather large. These states can therefore be considered as cluster states. As expected, the formal parameters (5.7) and

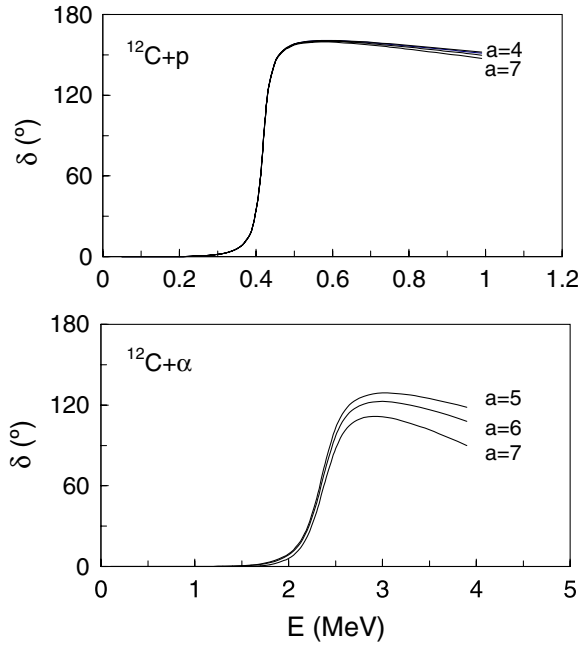


Figure 13. $^{12}\text{C} + \text{p}$ ($l = 0$) and $^{12}\text{C} + \alpha$ ($l = 1$) phase shifts in the single-pole R -matrix approximation computed with the parameters of table 10 for different channel radii.

(5.8) are strongly dependent on the channel radius. However, the corresponding phase shifts in figure 13 are very close to each other, in particular for the narrow resonance in $^{12}\text{C} + \text{p}$. For the broad resonance in $^{12}\text{C} + \alpha$, the phase shift is rather stable near the resonance energy, but more significant differences appear at higher energies. In such a case, the validity of the Breit–Wigner approximation is more limited. In other words, the single-pole approximation (5.3) should be replaced by an R matrix containing several terms.

5.3. Multiresonance elastic scattering

As mentioned above, the single-pole approximation is often valid at low energies. However, for nuclei with a high level density, several resonances may appear with the same angular momentum and parity. Then the interferences between different resonances and/or bound states in the same partial wave may be important. Typical examples are $^{12}\text{C} + \alpha$ or $^{14}\text{N} + \text{p}$ where several partial waves involve more than one state, even in a limited energy range.

In this case, the link between formal and observed parameters is more complicated, and was addressed for many years in a rather indirect way (see, for example, [14, 118]). More recently, an iterative procedure was proposed to determine the formal R -matrix parameters from observed values [23]. This method is valid for single-channel systems only. A generalization to multichannel problems was then developed by Brune [24]. The idea is to propose an alternative parametrization of the R matrix, where the input parameters are the observed data. It is based on the invariance of these values when the boundary parameters B_c (see (3.80)) are changed. We briefly summarize Brune’s method here, by assuming elastic scattering only. A more general presentation can be found in [24].

Let us assume N resonances in a given partial wave, with observed energies E_{Ri} and widths Γ_{Ri} . For each resonance, an observed reduced width is defined, according to (5.2), as

$$\gamma_{\text{obs},i}^2 = \Gamma_{Ri}/2P_l(E_{Ri}). \quad (5.11)$$

In the notations of [24], (5.7) is written as

$$\tilde{\gamma}_i^2 = \frac{\gamma_{\text{obs},i}^2}{1 - \gamma_{\text{obs},i}^2 S'_l(E_{Ri})}. \quad (5.12)$$

From these expressions, the formal pole energies E_n , used in the N -pole R -matrix expansion, are obtained from

$$N\mathbf{b}_n = E_n M \mathbf{b}_n, \quad (5.13)$$

where matrix elements N_{ij} and M_{ij} are given by

$$N_{ij} = \begin{cases} E_{Ri} + \tilde{\gamma}_i^2 S_l(E_{Ri}) & \text{for } i = j, \\ \tilde{\gamma}_i \tilde{\gamma}_j \frac{E_{Ri} S_l(E_{Rj}) - E_{Rj} S_l(E_{Ri})}{E_{Ri} - E_{Rj}} & \text{for } i \neq j, \end{cases} \quad (5.14)$$

and

$$M_{ij} = \begin{cases} 1 & \text{for } i = j, \\ -\tilde{\gamma}_i \tilde{\gamma}_j \frac{S_l(E_{Ri}) - S_l(E_{Rj})}{E_{Ri} - E_{Rj}} & \text{for } i \neq j. \end{cases} \quad (5.15)$$

The generalized eigenvalue problem (5.13) provides the formal energies E_n . The formal reduced width amplitudes γ_n are derived from the eigenvectors \mathbf{b}_n as

$$\gamma_n = \sum_{j=1}^N b_{n,j} \tilde{\gamma}_j. \quad (5.16)$$

When $N = 1$, it is easy to see that (5.7) and (5.8) are recovered. This method provides an efficient way to derive the R -matrix parameters. It represents the starting point of an alternative parametrization of the R matrix, proposed by Brune [24].

This formalism is illustrated in table 11 and figure 14 with the $^{14}\text{N} + \text{p}$ system. In the $J^\pi = 3/2^+$ partial wave ($l = 0$), we take three resonances into account. The observed values E_{Ri} and Γ_{Ri} [94] are given in table 11. As for the single-pole approximation, the formal parameters (E_n , γ_n) do depend on the channel radius. Figure 14 shows that the influence of a on the corresponding phase shifts is weak near the narrow resonance at 0.987 MeV (this resonance presents a small θ^2 value and has thus a complicated structure). As expected, this influence is more important in the vicinity of the broader states at 2.2 and 3.2 MeV.

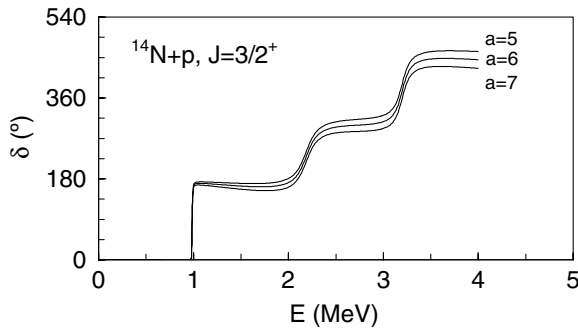
5.4. Phenomenological parametrization of multichannel collisions

To deal with inelastic or transfer cross sections, the R -matrix formalism must be extended to several channels. Rigorously this is even true in elastic scattering involving particles with non-zero spins. When the spins are different from zero, several (II) values (see (2.29)) are to be considered, each of them being characterized by a partial reduced width.

Let us consider the multichannel R matrix (3.86). In the calculable variant, the number of poles is equal to the product of

Table 11. R -matrix parameters (in MeV) with 3 poles for the $J^\pi = 3/2^+$, $l = 0$ partial wave in $^{14}\text{N} + \text{p}$.

Observed values		$a = 5$ fm	$a = 6$ fm	$a = 7$ fm
$E_{R1} = 0.987$	$\gamma_{\text{obs},1}^2$	0.0082	0.0054	0.0039
$\Gamma_{R1} = 0.00367$	$\theta_{\text{obs},1}^2$	0.0031	0.0029	0.0028
	γ_1^2	0.0097	0.0061	0.0042
	E_1	0.981	0.983	0.985
$E_{R2} = 2.187$	$\gamma_{\text{obs},2}^2$	0.114	0.086	0.069
$\Gamma_{R2} = 0.2$	$\theta_{\text{obs},2}^2$	0.043	0.047	0.050
	γ_2^2	0.119	0.089	0.070
	E_2	2.153	2.165	2.172
$E_{R3} = 3.209$	$\gamma_{\text{obs},3}^2$	0.053	0.042	0.034
$\Gamma_{R3} = 0.14$	$\theta_{\text{obs},3}^2$	0.020	0.023	0.025
	γ_3^2	0.051	0.041	0.034
	E_3	3.199	3.202	3.204

**Figure 14.** $^{14}\text{N} + \text{p}$ R -matrix phase shifts ($J^\pi = 3/2^+$) computed with the parameters of table 11.

the number of basis functions N by the number of channels. In the phenomenological approach, including all partial waves is often not realistic, since too many parameters may be involved. At low energies, the choice of the relative angular momentum l is guided by the penetration factor, i.e. the minimum l value for given J and π is often adopted. Such a selection mechanism does not exist for the channel spin I . In general, all possible values should be considered. The choice of the relevant partial waves is made according to the quality of the fit. For these reasons, the multichannel approach in the phenomenological variant of the R matrix is most often restricted to two channels.

Here we limit the presentation to a single pole at energy E_1 , the most frequently used approximation. In that case, the R matrix (3.86) is reduced to

$$R_{cc'}(E) = \frac{\gamma_c \gamma_{c'}}{E_1 - E}, \quad (5.17)$$

where γ_c is the reduced width amplitude of the pole in channel c (for simplicity we drop the index 1 of the reduced widths). These parameters are real. In this approximation, the property

$$R_{cc'}^2(E) = R_{cc}(E) R_{c'c'}(E), \quad (5.18)$$

provides the multichannel Z matrix (3.89) as

$$Z_{cc'} = (ak_c)^{-1/2} O_c [\delta_{cc'} - L_{c'} \sqrt{R_{cc} R_{c'c'}}]. \quad (5.19)$$

With the help of (B2), we obtain the inverse as

$$(Z^{-1})_{cc'} = (ak_c)^{1/2} O_c^{-1} \left[\delta_{cc'} + \frac{L_{c'} \sqrt{R_{cc} R_{c'c'}}}{1 - \sum_c R_{cc} L_c} \right], \quad (5.20)$$

where the logarithmic derivatives L_c (3.25) and outgoing functions O_c are defined for each channel. Using definition (3.88) for a real R matrix, one obtains

$$U_{cc'} = e^{i(\phi_c + \phi_{c'})} \left[\delta_{cc'} + 2i \frac{\sqrt{P_c P_{c'} R_{cc} R_{c'c'}}}{1 - \sum_c R_{cc} L_c} \right], \quad (5.21)$$

where ϕ_c is the hard-sphere phase shift (3.26) in channel c .

From the denominator in (5.21), the resonance energy and the reduced width are direct generalizations of (5.5) and (5.6),

$$E_R = E_1 - \frac{\sum_c \gamma_c^2 S_c(E_1)}{1 + \sum_c \gamma_c^2 S'_c(E_1)}, \quad (5.22)$$

$$\gamma_{\text{obs},c}^2 = \frac{\gamma_c^2}{1 + \sum_c \gamma_c^2 S'_c(E_1)}, \quad (5.23)$$

where index l in the penetration and shift factors is replaced by the more general channel index c . With (5.17), the collision matrix is parametrized at the generalized Breit-Wigner approximation [96] as

$$U_{cc'}^{\text{BW}} = e^{i(\phi_c + \phi_{c'})} \left[\delta_{cc'} + \frac{i \sqrt{\Gamma_c(E) \Gamma_{c'}(E)}}{E_R - E - i \Gamma(E)/2} \right], \quad (5.24)$$

where Γ_c is the observed partial width in channel c and $\Gamma = \sum_c \Gamma_c$. A simple calculation gives

$$\Gamma_c(E) = 2\gamma_{\text{obs},c}^2 P_c(E) \quad (5.25)$$

and $\Gamma_{cR} = \Gamma_c(E_R)$. Again, the R -matrix parameters (E_1, γ_c) can be deduced from the observed values as

$$\gamma_c^2 = \frac{\gamma_{\text{obs},c}^2}{1 - \sum_c \gamma_{\text{obs},c}^2 S'_c(E_R)}, \quad (5.26)$$

$$E_1 = E_R + \sum_c \gamma_c^2 S_c(E_R). \quad (5.27)$$

These analytical formulae are direct extensions of (5.7) and (5.8) obtained for elastic scattering in the single-pole approximation.

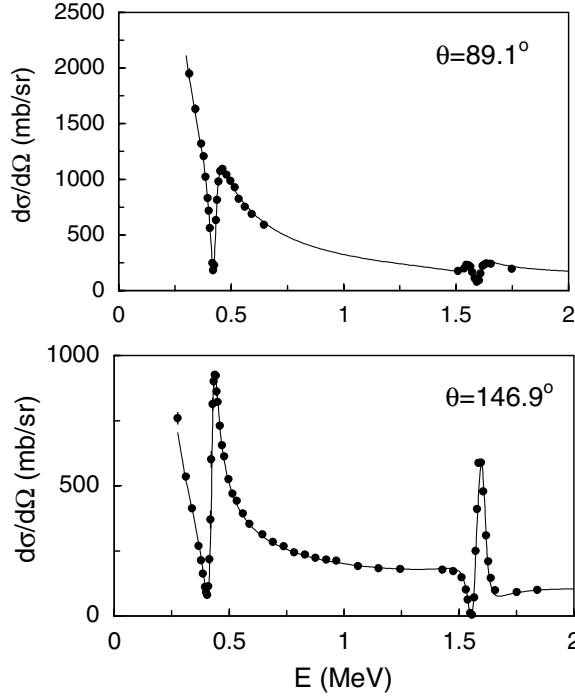
5.5. Application to the $^{12}\text{C} + \text{p}$ elastic scattering

Data on $^{12}\text{C} + \text{p}$ have existed for many years. In particular, elastic scattering cross sections have been measured with a high precision [119]. This system is well adapted to the phenomenological R -matrix approach, since the level density near threshold is quite low. This example should be considered as a typical application of the method. Similar fits have been done on the $^{16}\text{O} + \text{p}$ $l = 0$ elastic phase shifts [120] and on the $^{14}\text{O} + \text{p}$ cross section [48].

From [94], three resonances are expected in the energy range covered by the data: $1/2^+$ at 0.421 MeV, $3/2^-$ at 1.558 MeV and $5/2^+$ at 1.603 MeV. The pole corresponding to the bound state is neglected. Data sets at three c.m. angles ($\theta = 89.1^\circ, 118.7^\circ, 146.9^\circ$) are available. The smallest and largest angles are fitted simultaneously by using the single-pole approximation (5.3) for the resonant partial waves. For other partial waves, the hard-sphere phase shift is used. This

Table 12. R -matrix parameters from a simultaneous fit of $^{12}\text{C} + \text{p}$ scattering data [119] at $\theta = 89.1^\circ$ and 146.9° . Resonance energies E_R are expressed in MeV and widths Γ_R in keV.

	$J^\pi = 1/2^+$		$J^\pi = 3/2^-$		$J^\pi = 5/2^+$	
	E_R	Γ_R	E_R	Γ_R	E_R	Γ_R
$a = 4$ fm	0.427	33.8	1.560	51.4	1.603	48.1
$a = 5$ fm	0.427	32.9	1.559	51.4	1.604	48.1
$a = 6$ fm	0.427	30.9	1.558	51.3	1.606	47.8
Exp. [119]	0.424	33	1.558	55	1.604	50

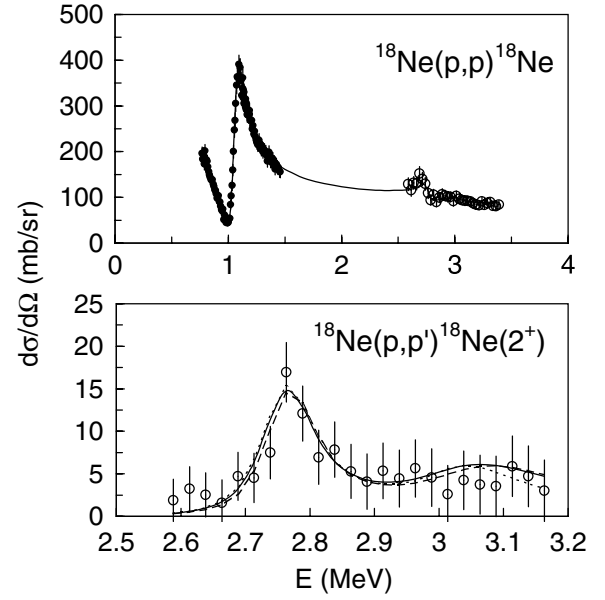
**Figure 15.** R -matrix fits of $^{12}\text{C} + \text{p}$ experimental excitation functions at two c.m. angles [119] with the parameters of table 12.

is consistent with the absence of resonance ($R_l = 0$), but plays a minor role in the cross sections. Replacing the hard-sphere phase shifts by zero provides essentially the same fits.

The observed resonance properties are given in table 12 for different channel radii. Clearly the results are almost independent of a , as expected from physical arguments. The fitted values are consistent with the literature [119], and the corresponding cross sections are shown in figure 15 for both scattering angles. The three channel radii provide fits which are indistinguishable at the scale of the figure. As expected [119], the R -matrix parametrization reproduces the data very well, not only in the vicinity of the resonances, but also between them, where the process is mostly non-resonant. This technique is very successful in the analysis of recent data involving radioactive beams (see, for example, [110–112]).

5.6. Application to the $^{18}\text{Ne}(\text{p},\text{p}')^{18}\text{Ne}(2^+)$ inelastic scattering

We present here an application of the phenomenological R -matrix method to inelastic scattering. The $^{18}\text{Ne}(\text{p},\text{p}')^{18}\text{Ne}(2^+)$ cross section has been measured in parallel with elastic cross sections [113]. These data

**Figure 16.** R -matrix fits of $^{18}\text{Ne}(\text{p},\text{p})^{18}\text{Ne}$ elastic (upper panel) and $^{18}\text{Ne}(\text{p},\text{p}')^{18}\text{Ne}(2^+)$ inelastic (lower panel) cross sections with the parameters of table 13. The data are from [121] (full circles) and [113] (open circles). The fits are done with $a = 4.5$ fm (dashed lines), $a = 5.0$ fm (solid lines) and $a = 5.5$ fm (dotted lines).

were obtained at various angles and complemented a previous data set, obtained at lower energies, and aimed at investigating elastic scattering only [121].

Here our goal is not to repeat the analysis of [113], where several angles were simultaneously included, but where previous elastic data were not considered. Instead, we select a single angle but cover a broader energy range by including data sets of [113, 121] in a global fit. Both experiments measured the elastic cross sections in different energy ranges, but also at slightly different angles. We select the elastic data sets of [113] at $\theta_{\text{lab}} = 6.2^\circ$ and of [121] at $\theta_{\text{lab}} = 4.9^\circ$. As the angular dependence is weak, we combine both these data sets at a common angle, taken as the average ($\theta_{\text{lab}} = 5.6^\circ$). For the inelastic cross section, the experimental angle [113] $\theta_{\text{lab}} = 6.2^\circ$ is used.

The experimental data and the corresponding R -matrix fits are presented in figure 16. As suggested in [113], the fits are performed by including three resonances ($J^\pi = 1/2^+, 5/2^+, 3/2^-$), which are characterized by their energy E_R and their partial widths Γ_1 and Γ_2 corresponding to the $\text{p} + ^{18}\text{Ne}(0^+)$ and $\text{p} + ^{18}\text{Ne}(2^+)$ channels, respectively. The fitted parameters are given in table 13 for different channel radii. As expected we essentially reproduce the results of [113, 121]. The $1/2^+$ resonance at 1.06 MeV is below the inelastic threshold ($\Gamma_2 = 0$), and corresponds to a single-particle state, with a large reduced width. The higher-lying resonances ($5/2^+, 3/2^-$) correspond to s states in the $\text{p} + ^{18}\text{Ne}(2^+)$ channel. They present a dominant width in that channel ($\Gamma_2 \gg \Gamma_1$) and correspond to a significant fraction of the Wigner limit (5.9). These resonances are hardly visible in the elastic data, and could not be properly analysed without the inelastic cross sections.

Owing to the use of a radioactive beam, the error bars are rather large in the inelastic cross sections, and the

Table 13. R -matrix parameters from a simultaneous fit of elastic and inelastic $^{18}\text{Ne} + p$ cross sections (see text). Resonance energies are given in MeV and widths in keV. The bracketed values represent the dimensionless reduced widths.

J^π		$a = 4.5 \text{ fm}$	$a = 5 \text{ fm}$	$a = 5.5 \text{ fm}$
$1/2^+$	E_R	1.064	1.063	1.062
	Γ_1	101 (0.26)	98 (0.23)	94 (0.20)
$5/2^+$	E_R	2.773	2.768	2.766
	Γ_1	7 (0.01)	6 (0.01)	7 (0.01)
	Γ_2	85 (0.46)	85 (0.40)	80 (0.34)
$3/2^+$	E_R	3.108	3.080	3.036
	Γ_1	11 (0.01)	11 (0.01)	9 (0.01)
	Γ_2	300 (0.47)	379 (0.57)	306 (0.48)
χ^2		0.43	0.44	0.54

sensitivity of the R -matrix parameters to the channel radius is slightly stronger than in $^{12}\text{C} + p$. In R -matrix analyses, this sensitivity should be taken into account in the evaluation of the recommended error bars.

5.7. Radiative-capture reactions

5.7.1. Extension of R -matrix formalism. The general formalism of radiative-capture reactions has been given in section 2.4. In the R -matrix theory, the matrix element \tilde{U} (2.58) is split into internal and external contributions as [21]

$$\tilde{U} = \tilde{U}_{\text{int}} + \tilde{U}_{\text{ext}}, \quad (5.28)$$

where we have dropped all indices for the sake of clarity. The terms \tilde{U}_{int} and \tilde{U}_{ext} of the rhs involve the internal and external wave functions, respectively. We assume here single-channel calculations, but the spins may be different from zero.

By using expansion (3.36) for the initial radial wave function $u_{l_i}^{\text{int}}$ and $C_{l_i} = 1$, the internal part of (2.58) becomes

$$\tilde{U}_{\text{int}} = \frac{e^{i(\delta_{l_i}^{J\pi} - \frac{\pi}{2})}}{|1 - L_{l_i} R_{l_i}^{J\pi}|} \sum_n \epsilon_n \frac{\sqrt{\Gamma_{\gamma,n}(E) \Gamma_n(E)}}{E_n - E}, \quad (5.29)$$

where we have introduced the formal gamma width of pole n as

$$\Gamma_{\gamma,n} = \frac{2J_f + 1}{2J + 1} \frac{8\pi(\lambda + 1)k_{\gamma,n}^{2\lambda+1}}{\lambda(2\lambda + 1)!!^2} |\langle \Psi^{J_f \pi_f} | | \mathcal{M}^{\sigma\lambda} | | \Phi_n^{J\pi} \rangle|^2 \quad (5.30)$$

with $k_{\gamma,n} = (E_n - E_f)/\hbar c$. The matrix element is calculated over the internal region only. Its definition involves a state $\Phi_n^{J\pi}$ corresponding to the pole E_n , whose radial part $r^{-1}\phi_n^{J\pi}(r)$ is defined as in the orthogonal basis (3.22) but for partial wave $J\pi$. Matrix element (5.29) depends on the particle width $\Gamma_n(E)$ (3.45) and on the gamma width at collision energy E ,

$$\Gamma_{\gamma,n}(E) = \left(\frac{E - E_f}{E_n - E_f} \right)^{2\lambda+1} \Gamma_{\gamma,n}(E_n) \quad (5.31)$$

(for simplicity, $\Gamma_{\gamma,n}(E_n)$ is often denoted as $\Gamma_{\gamma,n}$). In (5.29), $\epsilon_n = \pm 1$ is the product of the signs of the matrix element in (5.30) and of the reduced width amplitude. For a single-pole approximation, this sign does not play a role but determines interference effects in multi-resonance calculations.

The external contribution is determined as in (3.63). A calculation similar to the one leading to (2.64) provides

$$\begin{aligned} \tilde{U}_{\text{ext}} &= e Z_{\text{eff}}^{(E\lambda)} C_{l_f}^{J_f \pi_f} \frac{1}{(2J + 1)^{1/2}} (-1)^{l_f - J_f + \lambda} \left(\frac{2(\lambda + 1)k_\gamma^{2\lambda+1}}{\hbar v \lambda (2\lambda + 1)!!^2} \right)^{1/2} \\ &\times Z(l_i J l_f J_f, I_f \lambda) \int_a^\infty W_{l_f}(2\kappa_B r) r^\lambda (I_{l_i}(kr) - U_{l_i}^{J\pi} O_{l_i}(kr)) dr, \end{aligned} \quad (5.32)$$

where $C_{l_f}^{J_f \pi_f}$ is the ANC of the final bound state and $U_{l_i}^{J\pi}$ the collision matrix at energy E . This contribution is often referred to as ‘direct capture’. In fact, it is closely related to the internal term through the collision matrix. A resonant behaviour of the collision matrix affects the external term (5.32) (see also table 9). As usual, in the calculable R -matrix theory, the total matrix element (5.28) should not depend on the channel radius a , although each individual term does depend on a . In addition, one easily shows that both terms present an identical phase factor. The calculation can therefore be reduced to real expressions.

In the calculable R -matrix, the gamma width (5.30) is computed from basis functions. In the phenomenological variant, the constant $\Gamma_{\gamma,n}(E_n)$ appearing in (5.31) becomes a parameter. The treatment of radiative-capture reactions therefore requires one additional parameter for each pole, the gamma width $\Gamma_{\gamma,n}(E_n)$ (and the associated interference sign), and a global parameter, the ANC $C_{l_f}^{J_f \pi_f}$ of the final bound state. The latter parameter is sometimes available independently. As for elastic widths, the fitted values of the gamma widths may depend on the channel radius. The importance of this dependence will vary with the amplitude of the external contribution.

5.7.2. Isolated resonance approximation. Let us consider the single-pole approximation (5.3). Starting from expression (5.29) of the internal matrix element \tilde{U}_{int} , a simple calculation using definition (3.34) of the phase shift provides near the resonance energy E_R the approximation

$$\tilde{U}_{\text{int}}(E) \approx e^{i(\phi_{l_i} - \frac{\pi}{2})} \frac{\sqrt{\Gamma_{\gamma,R}(E) \Gamma_R(E)}}{E_R - E - i\Gamma_R(E)/2}, \quad (5.33)$$

where the observed particle width Γ_R is defined from (5.2) and where the observed gamma width $\Gamma_{\gamma,R}$ is given by

$$\Gamma_{\gamma,R}(E) = \frac{\Gamma_{\gamma,1}(E)}{1 + \gamma_1^2 S_1'(E_1)}. \quad (5.34)$$

The correction factor is thus identical for the particle and gamma widths (see (5.6)). For a resonant process, the main part of the wave function is located at short distances, and the external term (5.32) can often be neglected to a good approximation. In that case, the capture cross section (2.57) takes the usual Breit–Wigner form

$$\begin{aligned} \sigma_{J_f \pi_f, J\pi}^{\sigma\lambda}(E) &\approx \frac{\pi}{k^2} \frac{2J + 1}{(2I_1 + 1)(2I_2 + 1)} \frac{\Gamma_{\gamma,R}(E) \Gamma_R(E)}{(E_R - E)^2 + (\Gamma_R(E)/2)^2}. \end{aligned} \quad (5.35)$$

Table 14. Observed R -matrix parameters at the resonance energy E_R for the $^{12}\text{C}(p,\gamma)^{13}\text{N}$ reaction.

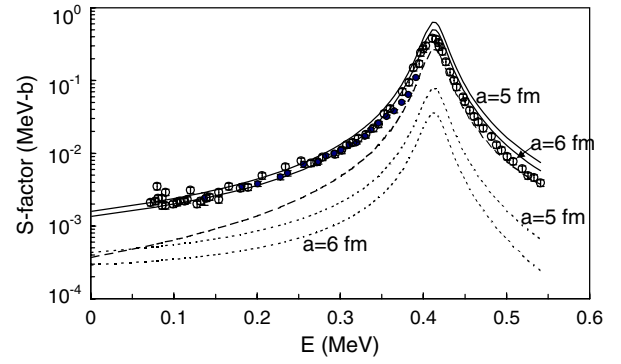
E_R (MeV)	Γ_R (keV)	$\Gamma_{\gamma,R}$ (eV)	C_1 (fm $^{-1/2}$)
0.415	31	0.4	1.1

As the electromagnetic interaction is weak, it is implicitly assumed that $\Gamma_{\gamma,R}(E) \ll \Gamma_R(E)$. This formula is of course an approximation which assumes that (i) there is no background or other resonances interfering and (ii) the external contribution is negligible. Going beyond these two approximations can be done by using the more general formulae (5.29) and (5.32). Note that the relative roles of \tilde{U}_{int} and \tilde{U}_{ext} depend on energy. When E becomes small, the internal part of the initial state becomes smaller and smaller, and the importance of the external contribution increases. The contribution of the external term also depends on the binding energy of the final state. If E_f is small, the asymptotic decrease in the bound-state wave function is slow and the external matrix element (5.32) may be important.

In the single-channel approximation, the internal and external components can be combined, which yields a slightly different definition for the gamma width [17]. In [122], the term involving the collision matrix in (5.32) is recast with the internal contribution. This provides modified electromagnetic matrix elements. As long as the external capture is negligible, all definitions of the gamma width are equivalent.

5.7.3. Application to $^{12}\text{C}(p,\gamma)^{13}\text{N}$. As discussed in section 4.12, the $^{12}\text{C}(p,\gamma)^{13}\text{N}$ S -factor at low energies is essentially determined by the properties of the $1/2^+$ ($l = 0$) resonance at $E_R = 0.42$ MeV in ^{13}N [17, 108]. As usual in nuclear astrophysics the main issue is to extrapolate the available data down to stellar energies (around 24 keV at the typical temperature 1.5×10^7 K). We use the phenomenological R -matrix approach with the single-pole approximation. In that case, four parameters are to be considered: the energy, proton width Γ_R , gamma widths $\Gamma_{\gamma,R}(E_R)$ of the resonance and the ANC C_{l_f} of the ^{13}N ground state ($J_f = 1/2^-$, $l_f = 1$). Since we are dealing with very low scattering energies and since ^{13}N is not strongly bound ($E_f = -1.94$ MeV), the ANC should be included. The fit is performed using (2.57), (5.32), (5.33) at a channel radius of $a = 5$ fm, and the resulting observed parameters are given in table 14.

Figure 17 presents the R -matrix S factor compared with experimental data. With the single-pole approximation the fit is not perfect, in particular above the resonance, where the R -matrix calculation slightly overestimates the data. This was already observed in figure 12, with the calculable approach. This problem has been addressed by Barker and Ferdous [17] who showed that an excellent fit of the data requires at least two poles in the R -matrix expansion. In addition to the total S factor, we also present the internal and external contributions independently. This analysis is done for $a = 5$ fm, but also for $a = 6$ fm, where the same observed parameters are used. The internal part (dashed line) corresponds to the Breit–Wigner approximation (5.35); it is almost insensitive to the choice of

**Figure 17.** $^{12}\text{C}(p,\gamma)^{13}\text{N}$ S -factor computed with the parameters of table 14 at $a = 5$ and 6 fm. The dashed line corresponds to the internal contribution ($a = 5$ fm and $a = 6$ fm are indistinguishable) and the dotted lines to the external term.

the channel radius. In contrast, the external part (dotted lines) does depend on a . Its influence near the resonance energy is weak but, as expected, it increases at low energies. Neglecting the external term when extrapolating down to stellar energies would provide a strong underestimation of the S factor.

6. Recent applications of the R -matrix method

6.1. Introduction

In section 4 we gave simple examples of the calculable R -matrix method, in order to illustrate the theoretical framework with applications which can be easily reproduced by the reader. However, in most cases, alternative methods, sometimes simpler, are available.

In this section, we present more ambitious applications of the R -matrix theory in nuclear physics. The first deals with microscopic cluster models [96], where the relative motion between the colliding particles is not defined by a potential, but by a nucleon–nucleon interaction. The R -matrix theory is also very efficient to solve coupled-channel problems [123]. In various models, the Schrödinger equation is reduced to a system of coupled differential equations. This can be solved, for example, with the generalized Numerov algorithm, but this method loses stability when the size of the system increases [124]. In that case, the R -matrix theory provides an efficient alternative, in particular when it is associated with the Lagrange-mesh method [93]. Two applications concerning the three-body continuum are presented: (i) the continuum discretized coupled channel (CDCC) method [87, 125] and (ii) the three-body hyperspherical formalism [83, 126, 127]. Recent applications of the R -matrix theory in atomic physics can be found, for example, in [72, 73, 128, 129].

6.2. Microscopic cluster models

6.2.1. General presentation. In nuclear physics, a microscopic theory is based on a description of all nucleons taking full account of antisymmetrization and derived from

interactions between nucleons. The Hamiltonian (2.25) reads

$$H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m_N} + \sum_{i>j=1}^A V_{ij} + \sum_{i>j>k=1}^A V_{ijk} - T_{\text{cm}}, \quad (6.1)$$

where A is the nucleon number, \mathbf{p}_i is the momentum of nucleon i and V_{ij} and V_{ijk} are two- and three-nucleon interactions. In (6.1), subtracting the center-of-mass energy T_{cm} guarantees that the wave function is free of spurious c.m. components [130]. The two-body interactions V_{ij} involve a nuclear term with spin-orbit, tensor and other components, and the Coulomb interaction. The three-body interactions V_{ijk} are necessary to explain the binding energies of the ^3H , ^3He and ^4He nuclei. Realistic interactions are derived from field theories and partly fitted on properties of the nucleon-nucleon system. For small nucleon numbers (i.e. $A \leq 4$), different techniques exist to find numerically exact solutions of the Schrödinger equation [131]. Few-body calculations can be performed by using various realistic interactions and compare well with experiment. For heavier systems, *ab initio* calculations [132, 133] become available. Different variants are being developed, but are currently limited to $A \approx 12$, and their application to continuum states is quite difficult [134, 135].

The microscopic cluster approach is based on an assumed cluster structure, i.e. on the existence of correlated subsystems in the fully antisymmetric wave function of the A -nucleon system [96]. The microscopic cluster model provides a unified framework for the description of nuclear spectroscopy and of nuclear reactions. The cluster assumption allows the application of a microscopic theory to heavier systems (typically up to $A \sim 20$ – 24), but requires the use of effective nucleon-nucleon two-body interactions (see, for example, [136, 137]) which are adapted to the cluster approximation. We use here the Minnesota effective interaction [137] which does not include tensor forces, but simulates their contribution in the binding energy of the deuteron by the central term. Three-body effects are in general also approximately simulated in these effective interactions.

6.2.2. The resonating group method. The resonating group method (RGM) assumes that the wave function can be expressed in terms of normed cluster wave functions ϕ_i involving A_i among the A nucleons and depending on translation-invariant internal coordinates, and of an unknown wave function $g_l(r)$ for their relative motion. Using the isospin formalism, the A -nucleon approximate wave function reads

$$\Psi_{lm} = \frac{A!}{A_1!A_2!} \mathcal{A} \phi_1 \phi_2 g_l(r) Y_l^m(\Omega), \quad (6.2)$$

where $\mathbf{r} = (r, \Omega)$ is the relative coordinate between the c.m. of the clusters and \mathcal{A} is the A -nucleon antisymmetrization projector

$$\mathcal{A} = \frac{1}{A!} \sum_{p=1}^{A!} (-1)^p P_p, \quad (6.3)$$

where the operator P_p performs a permutation among A particles. For simplicity, we assume a two-cluster

structure, with zero-spin clusters (see (2.32) for a multichannel definition). More general presentations can be found in [36, 37, 96, 138, 139]. The antisymmetric internal wave functions ϕ_1 and ϕ_2 are normalized to unity and defined in the harmonic-oscillator shell model, with a common oscillator parameter b [96]. First applications were limited to s-shell clusters [35], but progressively, heavier systems were considered [140, 141].

The unknown relative function $g_l(r)$ is obtained by solving the Schrödinger equation

$$H\Psi_{lm} = E\Psi_{lm}, \quad (6.4)$$

with Hamiltonian (6.1) and approximate wave function (6.2). By projecting the Schrödinger equation over $\langle \phi_1 \phi_2 Y_l^m(\Omega) |$, this technique provides an integro-differential equation involving local and non-local potentials [138]

$$(T_r + V_D(r) - E)g_l(r) + \int_0^\infty (\mathcal{K}_{HI}(r, r') - E\mathcal{K}_{NI}(r, r'))g_l(r') dr' = 0, \quad (6.5)$$

where T_r is the relative kinetic-energy operator (2.39), $V_D(r)$ is the direct potential (2.40) and $\mathcal{K}_{HI}(r, r')$ and $\mathcal{K}_{NI}(r, r')$ are the Hamiltonian and overlap exchange kernels, respectively.

At large distances, the Hamiltonian (6.1) can be written as

$$H \xrightarrow{r \rightarrow \infty} H_1 + H_2 + T_r + V_C(r), \quad (6.6)$$

where H_1 and H_2 are the internal Hamiltonians of the clusters, similar to (6.1), and $V_C(r)$ is the Coulomb potential between charges Z_1e and Z_2e . The internal energies E_i of clusters $i = 1, 2$ are defined by the variational expressions

$$E_i = \langle \phi_i | H_i | \phi_i \rangle. \quad (6.7)$$

In parallel, the wave function (6.2) tends to

$$\Psi_{lm} \xrightarrow{r \rightarrow \infty} \phi_1 \phi_2 g_l(r) Y_l^m(\Omega), \quad (6.8)$$

since the effect of the antisymmetrization operator \mathcal{A} is negligible when the nuclei do not overlap. For large r values, the radial wave function $rg_l(r)$ is given by the Coulomb equation (2.4). Although it is also suitable for bound states, the ansatz (6.2) of the total wave function is therefore well adapted to the treatment of scattering states.

The main problem of the RGM is not how to solve (6.5). This can be done by standard techniques, or by the R -matrix method [42]. Recent calculations, using realistic nucleon-nucleon interactions, have been performed on the $^3\text{He} + p$ and $^3\text{H} + n$ scattering [142] and on the α -nucleon scattering [135]. In these references, the RGM equation (6.5) is extended to a multichannel generalization. In [135], it is solved on a Lagrange mesh. The drawback of the RGM is that the calculation of the overlap and Hamiltonian kernels is not systematic. The reason is that the relative coordinate r and the cluster internal coordinates in (6.2) are modified in different ways by the terms of the antisymmetrizer \mathcal{A} . This method requires heavy analytical calculations [96, 138] (see also [42, 143] for examples of kernels). This problem is simplified by using the generator coordinate method (GCM), described in the next subsection.

6.2.3. *The generator coordinate method.* In the GCM, the relative wave function $g_l(r)$ is expanded over projected Gaussian functions [144] as

$$g_l(r) = \int f_l(R) \Gamma_l(r, R) dR, \quad (6.9)$$

where R is the generator coordinate and $\Gamma_l(r, R)$ is defined as

$$\Gamma_l(r, R) = \left(\frac{\mu_0}{\pi b^2} \right)^{3/4} \exp \left(-\mu_0 \frac{r^2 + R^2}{2b^2} \right) i_l \left(\frac{\mu_0 r R}{b^2} \right). \quad (6.10)$$

In this equation, μ_0 is the reduced mass in units of the nucleon mass, and $i_l(x) = \sqrt{\pi/2x} I_{l+1/2}(x)$, $I_{l+1/2}(x)$ being the modified spherical Bessel function of the first kind [49]. The calculation of $g_l(r)$ is therefore replaced by the calculation of the generator function $f_l(R)$.

Inserting (6.9) in the RGM definition (6.2) provides

$$\Psi_{lm} = \int f_l(R) \Phi_{lm}(R) dR, \quad (6.11)$$

where

$$\Phi_{lm}(R) = \frac{A!}{A_1! A_2!} \mathcal{A} \phi_1 \phi_2 \Gamma_l(r, R) Y_l^m(\Omega). \quad (6.12)$$

After multiplication by an appropriate factor depending on the c.m. coordinate of the A nucleons, the basis function $\Phi_{lm}(R)$ can be expressed as a projected Slater determinant provided that the oscillator parameters of the clusters are identical [144]. The Slater determinant is defined from A_1 and A_2 shell-model orbitals centred at $-A_2 R/A$ and $A_1 R/A$ for the first and second cluster, respectively. This property is well adapted to systematic and numerical calculations since it involves matrix elements of single-particle orbitals only. Well-known techniques exist to determine matrix elements between Slater determinants from single-particle matrix elements [145, 146]. They allow a rather simple extension of the cluster model to heavy systems [147] and to multichannel problems [148]. The projection over angular momentum l can be performed numerically [145].

In practice, the integral in (6.9) is replaced by a finite sum over a set of values R_n of the generator coordinate. This means that, at large distances r , the radial wave function $g_l(r)$ presents a Gaussian behaviour, not consistent with the physical asymptotic behaviour. This problem can be addressed by using the microscopic R -matrix method [36]. The wave function is approximated in the internal region by a discretized version of (6.11) as

$$\Psi_{lm}^{\text{int}} = \sum_{n=1}^N f_l(R_n) \Phi_{lm}(R_n). \quad (6.13)$$

In the external region, it is approximated by the asymptotic expression (6.8) as

$$\Psi_{lm}^{\text{ext}} = \phi_1 \phi_2 g_l^{\text{ext}}(r) Y_l^m(\Omega), \quad (6.14)$$

where the external radial function $rg_l^{\text{ext}}(r)$ is a linear combination of Coulomb functions, as in (3.3).

The application of the R -matrix method to the GCM is straightforward and follows the method detailed in section 3.2. The generalized matrix C defined in (3.14) involves matrix elements of the Hamiltonian in the internal region only. This is achieved by subtracting the external contributions [36]. By definition of the channel radius a , antisymmetrization effects and the nuclear interaction are negligible in the external region. The relevant matrix elements are therefore given by

$$\begin{aligned} \langle \Phi_l(R_n) | \Phi_l(R_{n'}) \rangle_{\text{int}} &= \langle \Phi_l(R_n) | \Phi_l(R_{n'}) \rangle \\ &\quad - \int_a^\infty \Gamma_l(r, R_n) \Gamma_l(r, R_{n'}) r^2 dr, \\ \langle \Phi_l(R_n) | H | \Phi_l(R_{n'}) \rangle_{\text{int}} &= \langle \Phi_l(R_n) | H | \Phi_l(R_{n'}) \rangle \\ &\quad - \int_a^\infty \Gamma_l(r, R_n) (T_r + V_C(r) + E_1 + E_2) \Gamma_l(r, R_{n'}) r^2 dr, \end{aligned} \quad (6.15)$$

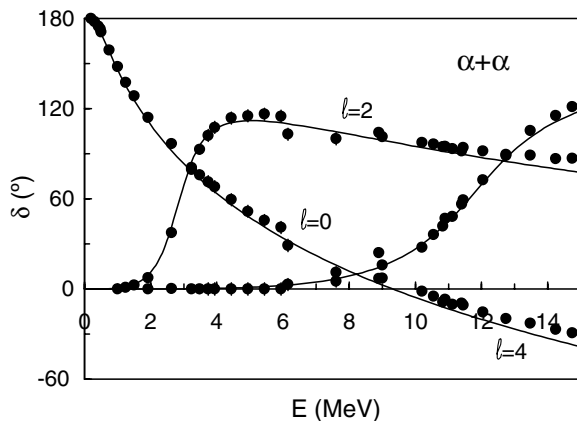
where the first terms in the rhs are matrix elements over the whole space, involving Slater determinants. The second terms represent the external contributions of the basis functions (6.10) and can easily be computed numerically. Then the R -matrix and the associated collision matrix are obtained as in section 3.2. Similarly, the collision matrix should not depend on the choice of the channel radius a , provided it is large enough to make the nuclear interaction and the antisymmetrization effects negligible in the external region. A generalization to multichannel systems can be found in [36, 37].

6.2.4. *Applications: $\alpha + \alpha$ and $^{12}\text{C} + \text{p}$.* We present three typical applications of the GCM associated with the microscopic R -matrix method. The first deals with the well-known $\alpha + \alpha$ phase shifts (see section 4.4). Then we compute the $^{12}\text{C} + \text{p}$ elastic cross section, as well as the $^{12}\text{C}(\text{p}, \gamma)^{13}\text{N}$ S factor at low energies. In all cases we use the Minnesota (MN) effective interaction [137] as central nucleon–nucleon force. The Minnesota potential provides the correct binding energy of the deuteron (without tensor force) and reproduces fairly well some properties of nucleon–nucleon scattering. It involves the admixture parameter u whose standard value is $u = 1$, but which can be slightly modified to fit important physical quantities, such as the energy of a bound state or of a resonance. For the $^{12}\text{C} + \text{p}$ system, a zero-range spin-orbit force (with amplitude S_0) is added [149].

The $\alpha + \alpha$ system is described by cluster wave functions ϕ_i defined from four 0s harmonic-oscillator orbitals with an oscillator parameter $b = 1.36$ fm for the two protons and the two neutrons. With the MN force, the binding energy of the α particle is 24.28 MeV, which is smaller than the experimental value of 28.30 MeV. This difference does not play an important role, since all theoretical energies are defined with respect to the $\alpha + \alpha$ threshold. The admixture parameter u is taken as $u = 0.94687$, as recommended in [143]. This value provides an excellent description of the $\alpha + \alpha$ phase shifts in a wide energy range. We use $N = 10$ basis functions in (6.13) with R_n values ranging from 0.8 to 8 fm by steps of 0.8 fm. In table 15, we give the 0^+ , 2^+ , 4^+ phase shifts at typical energies, and for various conditions of the calculation. The channel

Table 15. Microscopic $\alpha + \alpha$ phase shifts (in degrees) for different conditions of calculation.

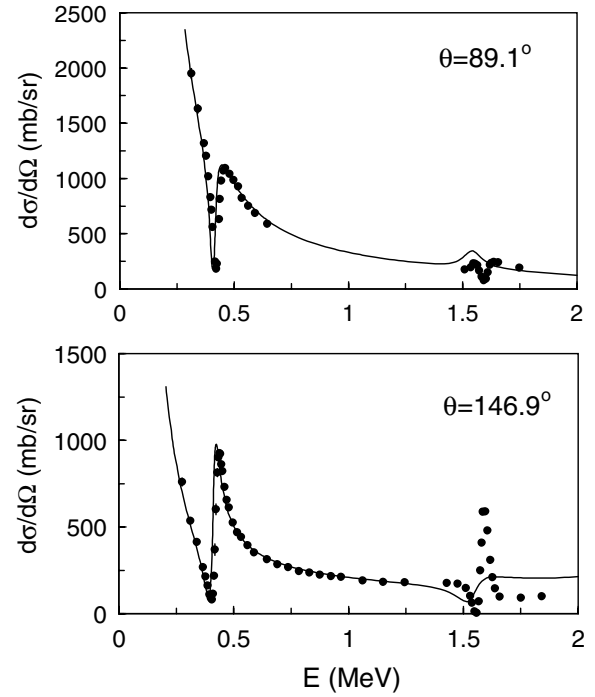
	E (MeV)	$N = 9$		$N = 10$	
		$a = 6.4$ fm	$a = 7.2$ fm	$a = 6.4$ fm	$a = 7.2$ fm
$l = 0$	1	146.00	145.93	146.00	146.00
	5	47.48	47.42	47.49	47.48
	10	-5.67	-5.79	-5.67	-5.67
	15	-38.47	-38.52	-38.46	-38.46
$l = 2$	1	0.56	0.53	0.56	0.56
	5	112.00	111.90	112.00	112.00
	10	94.97	94.94	94.98	94.97
	15	77.50	77.38	77.50	77.50
$l = 4$	1	0.00	0.00	0.00	0.00
	5	1.00	0.84	1.01	1.00
	10	26.66	26.64	26.66	26.65
	15	118.40	118.40	118.40	118.40

**Figure 18.** $\alpha + \alpha$ phase shifts with the microscopic cluster model. Experimental data are taken from [150].

radius a is taken as $a = 6.4$ fm or $a = 7.2$ fm, and $N = 9$ or 10 are considered. In all cases, the phase shifts are very stable when the conditions are changed. They can be obtained with an accuracy better than 0.1° . Figure 18 shows the phase shifts as a function of energy. It is known that a cluster model is well adapted to the $\alpha + \alpha$ system since the α particle has a large binding energy and since the first threshold (${}^7\text{Li} + p$) is near 17 MeV. The GCM phase shifts are therefore in very good agreement with experiment. The same results can be obtained from the RGM equation (6.5) [143].

The second application deals with the ${}^{12}\text{C} + p$ elastic scattering. The ${}^{12}\text{C}$ internal wave function ($b = 1.65$ fm) is described in the p shell limited to zero angular momentum and isospin. This provides four independent shell-model states defined from a linear combination of Slater determinants [151]. The calculation is therefore performed with four channels, obtained from the diagonalization of the ${}^{12}\text{C}$ basis. The first eigenstate corresponds to the ground state, and the three additional eigenvalues are considered as virtual excitations, which simulate the distortion of ${}^{12}\text{C}$ in the ${}^{12}\text{C} + p$ system.

The spin-orbit amplitude is fixed as $S_0 = 36.3$ MeV fm⁵, which allows us to reproduce the $1/2^-$ and $3/2^-$ binding energies of ${}^{13}\text{N}$ with $u = 0.77$. This value is used for negative-parity partial waves. In positive parity, $u = 0.998$ reproduces

**Figure 19.** ${}^{12}\text{C} + p$ excitation functions at two c.m. angles. The data are from [119].

the experimental energy of the $1/2^+$ resonance. The GCM widths of the $1/2^+$ and $3/2^-$ resonances are 43 keV and 99 keV, somewhat larger than the experimental values (31.7 ± 0.8 keV and 62 ± 4 keV, respectively [94]).

The ${}^{12}\text{C} + p$ excitation functions at $\theta = 89.1^\circ$ and $\theta = 146.9^\circ$ are shown in figure 19. Below 1.5 MeV, the agreement with experiment is quite good. However, the resonant structure near 1.6 MeV is not well described since the experimental data involve a $5/2^+$ resonance, which cannot be described with a simple cluster structure. This problem often occurs in microscopic cluster models, where some experimental states do not have a cluster structure, and are therefore not present in the model (see, for example, [152] for the ${}^{16}\text{O} + p$ system). Of course the phenomenological approach (see figure 15) provides a better description, but the parameters are adjusted to the data, and all resonances are included from the very beginning.

Our third application of the GCM is the ${}^{12}\text{C}(p, \gamma){}^{13}\text{N}$ cross section at astrophysical energies. The matrix elements of the $E1$ operator are determined as explained in section 5.7.1 (see [37] for detail). The capture cross section requires the ${}^{13}\text{N}$ ground-state wave function, as well as ${}^{12}\text{C} + p$ scattering states. Only s waves, corresponding to the $1/2^+$ resonant partial wave, are included in the scattering state. Calculations with d waves show that this component is of the order of 15% at 1 MeV, but becomes negligible as soon as the energy decreases, because of the higher centrifugal barrier.

The resulting S factor (2.55) is shown in figure 20. As expected from the overestimation of the proton width, the peak near the $1/2^+$ resonance at 0.42 MeV is slightly too broad. This type of calculation cannot be expected to perfectly reproduce the data. However, the S factor is quite satisfactory considering the fact that no parameter is fitted to capture data. The model has thus a predictive power which is very useful for

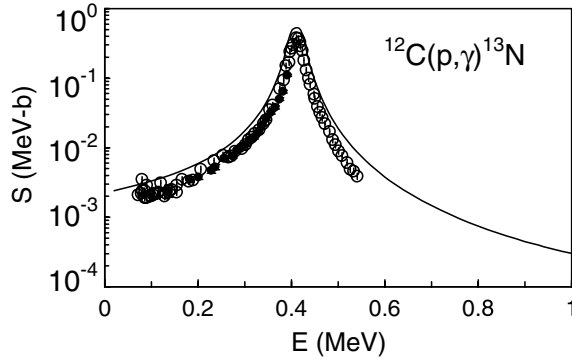


Figure 20. $^{12}\text{C}(p,\gamma)^{13}\text{N}$ GCM S -factor. The experimental data are from [107] (open circles) and [108] (closed circles).

capture reactions that have not been measured yet or cannot be measured. The GCM has been used to study many reactions of astrophysical interest, to compute either the cross section or the properties of low-energy resonances (see, for example, [153]).

6.3. The continuum discretized coupled channel (CDCC) method

6.3.1. Formalism. The purpose of the CDCC method is to determine, as accurately as possible, the scattering and dissociation cross sections of a nucleus which can be easily broken up in the nuclear or Coulomb field of a target. The final states may thus involve several particles: the target and the fragments of the projectile. The relative motion of these fragments is described by approximate continuum wave functions at discrete energies. The CDCC method was suggested by Rawitscher [125] and first applied to deuteron + nucleus elastic scattering and breakup reactions. It was then extensively developed and used by several groups [87, 124]. Interest has been further revived by the availability of radioactive beams of weakly bound nuclei dissociating into three fragments, such as ^6He whose first dissociation channel is $\alpha + n + n$ [154, 155]. Although variants of the CDCC method also exist in atomic physics [156], we focus here on applications in nuclear physics with two-body projectiles. To simplify the presentation, we assume a spin zero for the constituents of the projectile, and for the target t . As usual in CDCC calculations, the internal structure of the three particles is neglected.

Let us consider the coordinate system of figure 21: \mathbf{R} is the internal coordinate of the projectile and \mathbf{r} is the coordinate of the relative motion between projectile and target. The three-body Hamiltonian is given by

$$H = H_0 + T_r + V_{t1} \left(\mathbf{r} + \frac{A_2}{A} \mathbf{R} \right) + V_{t2} \left(\mathbf{r} - \frac{A_1}{A} \mathbf{R} \right), \quad (6.16)$$

where H_0 is the two-body Hamiltonian of the projectile

$$H_0 = T_R + V_{12}(R), \quad (6.17)$$

and A_1 and A_2 are the masses of the fragments ($A = A_1 + A_2$).

In general, potential $V_{12}(R)$ associated with the projectile is real, whereas the interactions V_{ti} between the fragments i

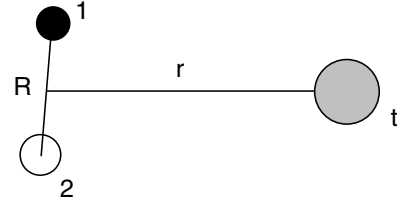


Figure 21. Coordinate system used for CDCC three-body calculations.

and the target t are derived from the optical model, and thus complex. In a schematic notation, the wave function associated with (6.16) can be expanded as

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum_B \Phi_B(\mathbf{R}) u_B(\mathbf{r}) + \int \Phi_k(\mathbf{R}) u_k(\mathbf{r}) dk, \quad (6.18)$$

where B denotes the bound states of the projectile and $\phi_k(\mathbf{R})$ are two-body scattering wave functions with wave number k . The first term represents the elastic and inelastic channels and the second term is associated with the breakup contribution.

In practice, two methods are available to perform the continuum discretization, i.e. to discretize the integral over k . In the ‘pseudo-state’ approach, it is replaced by a sum over square-integrable positive-energy eigenstates of Hamiltonian (6.17). The projectile Hamiltonian H_0 is diagonalized over a finite basis, yielding the square-integrable radial functions $\Phi_i^L(\mathbf{R})$ at energies E_i^L ,

$$H_0 \Phi_i^L(\mathbf{R}) Y_L^M(\Omega_R) = E_i^L \Phi_i^L(\mathbf{R}) Y_L^M(\Omega_R). \quad (6.19)$$

These functions are associated with bound states ($i = B$, $E_i < 0$), or represent square-integrable approximations of continuum wave functions ($E_i > 0$).

The alternative is to replace the integral over k by averages of exact scattering states over a range of energies (‘bin’ method) [87]. This approach also provides square-integrable basis functions. As far as the applicability of the R -matrix is concerned, both methods are treated in the same way. We use here the pseudo-state method.

The total wave function (6.18) is then rewritten, for an angular momentum J and parity $\pi = (-1)^{l+L}$, as

$$\Psi^{JM\pi}(\mathbf{r}, \mathbf{R}) = \sum_{lLi} Y_{lL}^{JM}(\Omega_r, \Omega_R) \Phi_i^L(\mathbf{R}) u_{lLi}^{J\pi}(r), \quad (6.20)$$

where J results from the coupling of orbital momenta l and L , and

$$Y_{lL}^{JM}(\Omega_r, \Omega_R) = i^{l+L} [Y_l(\Omega_r) \otimes Y_L(\Omega_R)]^{JM}. \quad (6.21)$$

The relative wave functions $u_{lLi}^{J\pi}(r)$ are given by a set of coupled equations

$$\begin{aligned} & \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) + E_i^L - E \right] u_c^{J\pi}(r) \\ & + \sum_{c'} V_{cc'}^{J\pi}(r) u_{c'}^{J\pi}(r) = 0, \end{aligned} \quad (6.22)$$

where the channel index c stands for (lLi) . Of course, the sum over L must be truncated at some value L_{\max} . The sum over

the pseudo-states i is limited by the number of basis states and can be reduced further by eliminating states above a maximum energy E_{\max} . The CDCC problem is therefore equivalent to a system of coupled equations where the potentials $V_{cc'}^{J\pi}(r)$ are given by

$$V_{cc'}^{J\pi}(r) = \langle Y_{iL}^{JM}(\Omega_r, \Omega_R) \Phi_i^L(R) | V_{t1} \left(r + \frac{A_2}{A} \mathbf{R} \right) + V_{t2} \left(r - \frac{A_1}{A} \mathbf{R} \right) | Y_{i'L'}^{JM}(\Omega_r, \Omega_R) \Phi_{i'}^{L'}(R) \rangle. \quad (6.23)$$

This matrix element represents a 5-dimensional integral over (Ω_r, Ω_R, R) . In practice the potentials are expanded into multipoles as

$$V_{t1} \left(r + \frac{A_2}{A} \mathbf{R} \right) + V_{t2} \left(r - \frac{A_1}{A} \mathbf{R} \right) = \sum_{\lambda} V_{\lambda}(r, R) P_{\lambda}(\cos \theta_{Rr}), \quad (6.24)$$

where θ_{Rr} is the angle between \mathbf{R} and \mathbf{r} , and $P_{\lambda}(x)$ a Legendre polynomial. In practice the number of λ values is limited by angular momentum couplings. The four angular integrals in (6.23) are performed analytically, whereas the integration over R may require a numerical approach.

System (6.22) can be solved by various methods [123], in particular with the R -matrix formalism. We expand the radial wave functions $u_c^{J\pi}(r)$ over Lagrange functions (4.7), and the calculation of potential (6.23) is therefore limited to the mesh points as in (4.12). Further simplifications are possible by describing the projectile wave functions $\Phi_i^L(R)$ (see (6.19)) in a Lagrange basis as well. In this well-known two-body problem [93], the wave function is expanded in a basis differing from (4.7) by the fact that it is constructed from Laguerre polynomials. The matrix elements involving $\Phi_i^L(R)$ (as, for example, in the potentials (6.23)) are determined in a fast and accurate way. The extension to three-body projectiles [154, 155] can also be considered in this approach. The calculations are much more time-consuming since the projectile wave functions depend on two radial coordinates, and are more difficult to handle. Consequently, even though the formulation is similar, the calculation of the potential matrix elements (6.23) raises important numerical difficulties, which can be addressed by the present technique.

6.3.2. Application to the $d + {}^{58}\text{Ni}$ elastic scattering. The CDCC theory, associated with the R -matrix method, is applied to the elastic scattering of deuterons on ${}^{58}\text{Ni}$ at $E_{\text{lab}} = 80$ MeV. This collision has been widely covered in the literature [87, 157]. The $p + n$ and nucleon- ${}^{58}\text{Ni}$ interactions are chosen as in these references.

The first step is to determine the deuteron ground state, and the $p + n$ pseudo-states, from (6.19). These wave functions are expanded over a Lagrange–Laguerre basis, involving a scaling parameter h which is adapted to the size of the system [93]. Typical values are $h \sim 0.3\text{--}0.4$ fm with 15–20 basis functions. We include partial waves $L = 0, 2, 4$. In a second step, the potentials $V_{cc'}(r)$ (see (6.23)) are computed at the mesh points of the $d + {}^{58}\text{Ni}$ relative motion. These mesh points are defined

Table 16. Amplitudes $\eta^{J\pi}$ and phase shifts $\delta^{J\pi}$ (in degrees) for elastic $d + {}^{58}\text{Ni}$ elastic scattering ($L_{\max} = 4$, $E_{\max} = 40$ MeV) for $J^{\pi} = 0^{+}$ and 17^{-} .

a (fm)	N	η^{0+}	δ^{0+}	η^{17-}	δ^{17-}
15	30	0.117	31.5	0.5958	20.454
17	30	0.105	29.7	0.5958	20.454
15	40	0.116	31.2	0.5958	20.454
17	40	0.116	31.1	0.5959	20.454
[157]				0.5956	19.9

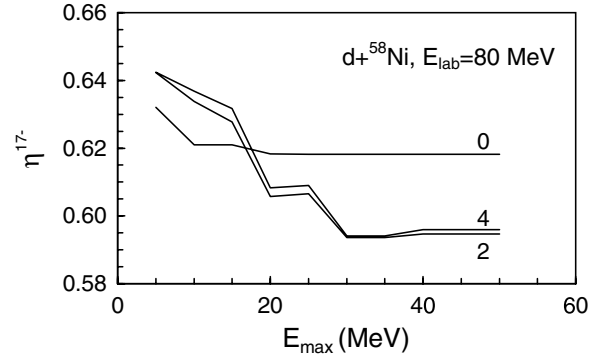


Figure 22. Amplitude η^{17-} for different L_{\max} values (labels) as a function of the truncation energy E_{\max} .

from the channel radius a and from the size of the basis N (see (4.8)).

In table 16 and figure 22, we present the elastic part of the collision matrix

$$U_{11}^{J\pi} = \eta^{J\pi} \exp(2i\delta^{J\pi})$$

for $J^{\pi} = 0^{+}$ and 17^{-} . Values for $J^{\pi} = 17^{-}$ can be compared with the literature [157]. The amplitude η and phase shift δ are computed for different channel radii and numbers of wave functions. For the pseudo-states, we truncate at $L_{\max} = 4$ and $E_{\max} = 50$ MeV. The number of pseudo-states depends on the size of the basis (here, typically their number is about 20). We have checked that changing the size of the basis does not affect the phase shifts. Table 16 shows that, for high partial waves ($J^{\pi} = 17^{-}$), the stability with the numerical conditions is virtually perfect. The amplitude is in excellent agreement with [157], but the phase shift is slightly different (0.5°). For low partial waves ($J^{\pi} = 0^{+}$), the stability is still acceptable but higher N values are necessary. This can be understood by the fact that the internal part is more and more important as J decreases.

Figure 22 displays the amplitude η^{17-} as a function of the $p + n$ truncation energy E_{\max} , and for different L_{\max} values. The convergence with respect to E_{\max} is reached near $E_{\max} \approx 40$ MeV, which corresponds to $k_{\max} \approx 1$ fm $^{-1}$. This result agrees with the conclusion of [157]. From the figure, it is clear that $L = 0$ pseudo-states are not sufficient to provide accurate values. However, a very good convergence is already obtained with $L_{\max} = 2$.

The elastic cross section is presented in figure 23, and compared with experimental data (quoted in [158]). A first calculation, referred to as a ‘no-breakup’ approximation, is

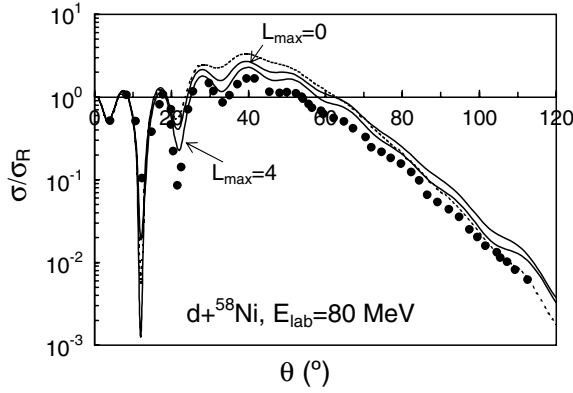


Figure 23. $d + {}^{58}\text{Ni}$ elastic cross section relative to the Rutherford cross section at $E_{\text{lab}} = 80$ MeV. Solid lines correspond to $E_{\text{max}} = 40$ MeV and to $L_{\text{max}} = 0, 4$. The dotted line corresponds to the no-breakup approximation. Experimental data are taken from [158].

done by including only the ground state of the deuteron (dotted line). This approximation clearly overestimates the data above 30° . With $L = 0$ deuteron pseudo-states, the agreement in the region 30° – 50° is significantly improved. The present result is very close to the CDCC calculation of [158]. The curves with $L_{\text{max}} = 2$ and $L_{\text{max}} = 4$ are indistinguishable at the scale of the figure.

From this example, it turns out that the R -matrix method is a very efficient tool to solve the CDCC equations. By using Lagrange functions, the calculation of the coupling potentials $V_{cc'}(r)$ is very fast, since only values at the mesh points are required (typically $N \sim 30$ – 40). Consequently, the main part of the computer time is devoted to the inversion of the (complex) matrix C (see (3.15)). Fast techniques are available for matrix inversion, and the total computer time is therefore very short (typically a few seconds for the angular distribution of figure 23). This opens encouraging perspectives for CDCC calculations involving three-body projectiles which require large computer times with standard techniques [154, 155].

6.4. Three-body continuum states

6.4.1. Hyperspherical formalism. The separation energy being very low in exotic nuclei, a precise treatment of the continuum is necessary for the description of reactions leading to a three-body dissociation. The R -matrix method provides an efficient way to treat three-body continuum states [83, 127]. We use the hyperspherical formalism, well adapted to three-body systems [88, 126, 159]. This model is well known, and is just briefly outlined here.

In a three-body system, the Hamiltonian is defined, after removal of the c.m. motion, as

$$H = \sum_{i=1}^3 T_i - T_{\text{cm}} + \sum_{i>j=1}^3 V_{ij}(\mathbf{r}_j - \mathbf{r}_i), \quad (6.25)$$

where \mathbf{r}_i are the space coordinates of the particles, T_i their kinetic energy and V_{ij} the interaction between particles i and j . The scaled Jacobi coordinates $\mathbf{x} = (\mathbf{x}, \Omega_x)$ and

$\mathbf{y} = (\mathbf{y}, \Omega_y)$ are defined from the coordinates \mathbf{r}_i , and provide the hyperradius ρ and hyperangle α as

$$\rho = \sqrt{x^2 + y^2},$$

$$\alpha = \arctan(y/x). \quad (6.26)$$

In this coordinate system, the 3-body kinetic energy involves the operator K^2 which generalizes the concept of angular momentum in 2-body systems. It commutes with l_x^2 and l_y^2 and their common eigenfunctions $\mathcal{Y}_{\gamma K}^{JM}(\Omega_5)$ are known analytically (see [88] for details). The eigenvalue of K^2 is $K(K+4)$ where the integer K is the hypermomentum quantum number. In these expressions, $\Omega_5 = (\Omega_x, \Omega_y, \alpha)$ and γ stands for $\gamma = (l_x, l_y, L, S)$ where (l_x, l_y) are the angular momenta associated with (x, y) , L and S are the total orbital momentum and spin, respectively. The total angular momentum J results from the coupling of L and S , and the parity is given by $\pi = (-1)^K$.

The wave function of partial wave $J\pi$ associated with Hamiltonian (6.25) is then expanded over hyperspherical harmonics as

$$\Psi^{JM\pi}(\rho, \Omega_5) = \rho^{-5/2} \sum_{\gamma K} \chi_{\gamma K}^{J\pi}(\rho) \mathcal{Y}_{\gamma K}^{JM}(\Omega_5), \quad (6.27)$$

where the radial functions $\chi_{\gamma K}^{J\pi}(\rho)$ have to be determined. The Schrödinger equation is then reduced to a system of coupled differential equations

$$\left[-\frac{\hbar^2}{2m_N} \left(\frac{d^2}{d\rho^2} - \frac{(K+3/2)(K+5/2)}{\rho^2} \right) - E \right] \chi_{\gamma K}^{J\pi}(\rho) + \sum_{K'\gamma'} V_{K'\gamma', K\gamma}^{J\pi}(\rho) \chi_{\gamma' K'}^{J\pi}(\rho) = 0, \quad (6.28)$$

where the potentials matrix elements are defined as

$$V_{K'\gamma', K\gamma}^{J\pi}(\rho) = \langle \mathcal{Y}_{\gamma' K'}^{JM}(\Omega_5) | \sum_{i>j=1}^3 V_{ij}(\mathbf{r}_j - \mathbf{r}_i) | \mathcal{Y}_{\gamma K}^{JM}(\Omega_5) \rangle. \quad (6.29)$$

The integrals over Ω_x and Ω_y are performed analytically, whereas a numerical quadrature is used for the integral over the hyperangle α . With the Raynal–Revai coefficients [160, 161] the evaluation of (6.29) is rather easy. A truncation must be done in the summation over K ; this provides a maximum K value, denoted as K_{max} . The number of components in (6.27) increases rapidly when K_{max} increases.

This formalism has been extensively applied to three-body bound states [88]. In [162], we have addressed this problem by expanding the radial wave functions over Lagrange functions. This approach provides a very fast method to evaluate matrix elements (6.29).

One of the main issues associated with nuclear three-body problems is the presence of forbidden states in the nucleus–nucleus interaction [96, 98]. These two-body forbidden states introduce spurious states in the three-body problem and should be removed. This problem has been discussed in detail by Thompson *et al* [127], and is usually solved, either by introducing a projector over the forbidden states [163] or by using supersymmetric potentials [164].

6.4.2. The R -matrix method for three-body states. The treatment of three-body states, with exact three-body asymptotic conditions, is more recent [83, 127]. In the R -matrix method, the solutions of system (6.28) are split into two regions,

$$\chi_{\gamma K, \text{int}}^{J\pi}(\rho) = \sum_{i=1}^N c_{\gamma Ki}^{J\pi} \varphi_i(\rho), \quad (6.30)$$

for $\rho < a$ where $\varphi_i(\rho)$ are basis functions and

$$\chi_{\gamma K, \text{ext}}^{J\pi}(\rho) = C_{\gamma K}^{J\pi} [H_{\gamma K}^{-}(k\rho) \delta_{\gamma\gamma'} \delta_{KK'} - U_{\gamma K, \gamma' K'}^{J\pi} H_{\gamma K}^{+}(k\rho)] \quad (6.31)$$

for $\rho \geq a$. In this equation, $k = \sqrt{2m_N E/\hbar^2}$, $C_{\gamma K}^{J\pi}$ is a normalization coefficient, $U^{J\pi}$ is the three-body collision matrix and the incoming and outgoing functions $H_{\gamma K}^{\pm}(x)$ are defined as

$$H_{\gamma K}^{\pm}(x) = \pm i \left(\frac{\pi x}{2} \right)^{1/2} [J_{K+2}(x) \pm i Y_{K+2}(x)],$$

where $J_n(x)$ and $Y_n(x)$ are Bessel functions of first and second kind, respectively. We assume here systems without two-body Coulomb interaction.

As in previous applications, we choose Lagrange functions for the basis states $\varphi_i(\rho)$ [83]. The R -matrix method is then used to solve the coupled system (6.28). Formally this is equivalent to the CDCC system (see (6.22)), although the external wave function involves Bessel functions. Another difference arises from the long range of the three-body potential (6.29). As shown in [83], this potential behaves as

$$V_{K'\gamma', K\gamma}^{J\pi}(\rho) \rightarrow \frac{V_{0, K'\gamma', K\gamma}^{J\pi}}{\rho^3}, \quad (6.32)$$

even with short-range two-body interactions. This arises from the definition of the hyperspherical coordinates. Even for large ρ values, two particles can still be close to each other and interact strongly. Constants $V_{0, K'\gamma', K\gamma}^{J\pi}$ can take rather large values (examples are given in [83]). For this reason, the R -matrix radius should take large values (typically $a \sim 200$ – 300 fm) to ensure that potential (6.32) is negligible compared with the centrifugal term in (6.28). In those conditions, the propagation techniques described in section 3.9 are necessary to avoid huge basis sizes.

6.4.3. Application to $\alpha + n + n$ three-body scattering. The ${}^6\text{He}$ nucleus is an ideal test case for three-body continuum states and has been considered in previous studies [83, 127]. Accurate $\alpha + n$ and $n + n$ interactions exist in the literature [137, 165]. The $\alpha + n$ subsystem presents one forbidden state for $l = 0$, which is removed by using a pair of supersymmetric transformations [164]. Details can be found in [83].

Figure 24 illustrates the need for propagation techniques. Dotted lines correspond to channel radii $a = 20$ fm and $a = 30$ fm, and are compared with the exact values (solid line, $a = 250$ fm) obtained by propagation. As expected from the long range of the three-body potential (6.29), large values for the channel radius are necessary. As soon as this condition

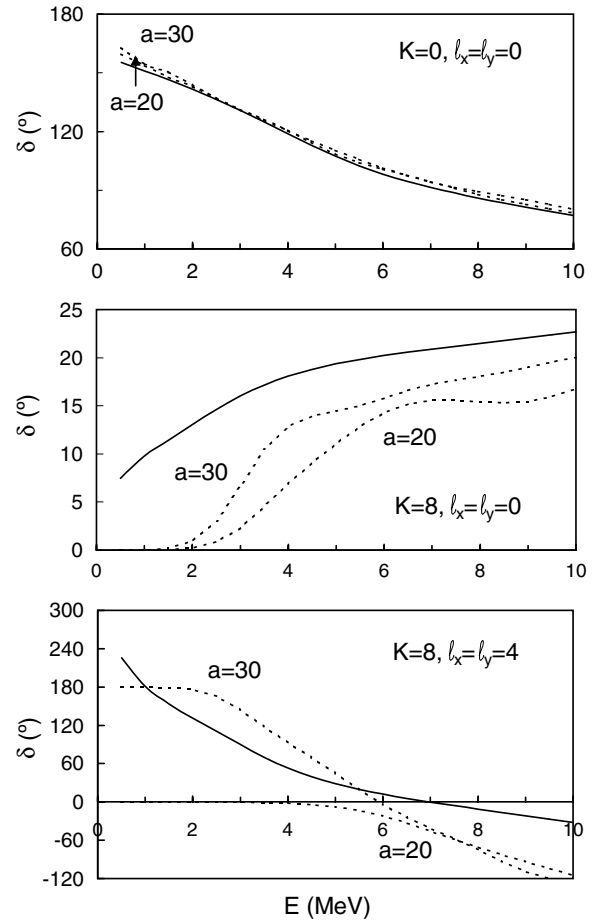


Figure 24. $\alpha + n + n$ phase shifts ($J^\pi = 0^+$) for channel radii $a = 20$ fm ($N = 20$) and $a = 30$ fm ($N = 30$) without propagation (dashed lines). Solid lines are obtained with propagation up to $a = 250$ fm. Reprinted from [83], copyright (2006), with permission from Elsevier.

is satisfied, the R -matrix phase shifts are very stable against variations of a .

In figure 25, we display the 0^+ eigenphases as a function of K_{max} . The eigenphases are obtained after diagonalization of the collision matrix (see (2.37)). In each case we select the eigenphase with the dominant resonant structure. Above 4 MeV, a fair convergence is obtained, but high hypermomenta are necessary near 2 MeV. The 0^+ , 1^- , 2^+ eigenphases are displayed in figure 26 with $K_{\text{max}} = 24, 19$ and 16 , respectively. The 2^+ phase shift presents an experimentally well-known narrow resonance at low energies. For the 0^+ and 1^- partial waves, the calculation shows a broad structure near 1.5 MeV. The existence of three-body resonances at low energies, and in particular for $J^\pi = 1^-$, is still an open debate (see, for example, the discussion in [166]), from the experimental as well as from the theoretical viewpoints.

In the future, this formalism could be applied to the 3α system. Current experimental [167] and theoretical [168–170] results are rather controversial concerning the existence (or non-existence) of broad 0^+ and 2^+ resonances above the 3α threshold. This issue is crucial in nuclear astrophysics, since the Hoyle state (0_2^+) in ${}^{12}\text{C}$ is known to be the main resonance in Helium burning. If the properties of this resonance are

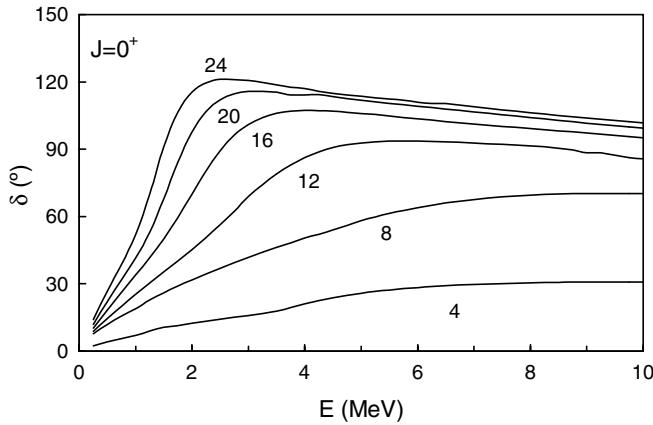


Figure 25. Energy dependence of $\alpha + n + n$ eigenphases ($J^\pi = 0^+$) for different K_{\max} values. Reprinted from [83], copyright (2006), with permission from Elsevier.

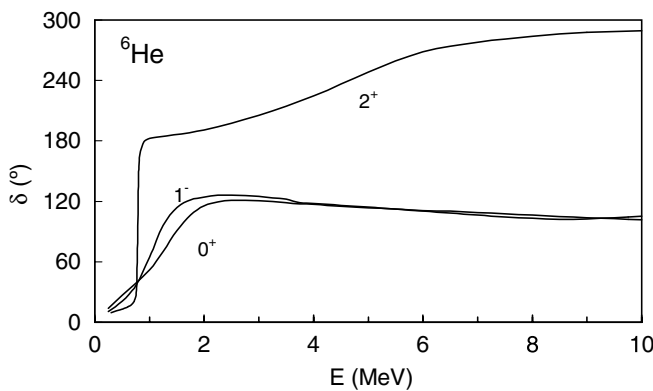


Figure 26. Eigenphases of ${}^6\text{He}$ for different J^π values. Reprinted from [83], copyright (2006), with permission from Elsevier.

well known, the ${}^{12}\text{C}$ level scheme above this resonance is still not clear. In this context, the calculation of 3α phase shifts would help clarify the situation. However, existing $\alpha + \alpha$ local potentials do not provide a satisfactory description of the ${}^{12}\text{C}$ spectroscopy [171]. Non-local potentials are more promising [171, 172], but although bound states can be easily investigated with Lagrange meshes [83], their application to three-body continuum states remains a challenge for the future.

7. Conclusion

The R -matrix method was born sixty years ago with the important but rather limited goal of describing resonances in nuclear reactions. Today it has evolved into powerful tools covering several subfields of atomic, molecular and nuclear collisions. The literature is so enormous that it is not possible to master it and to cover it in a single review.

We have emphasized a fact that is often unknown to R -matrix practitioners: two variants exist. The phenomenological R matrix remains close to the original spirit and is very much used in nuclear physics to parametrize low-energy cross sections. Its main merits are that all parameters are real and that they have a physical meaning. Although resonances often play a crucial role in these parametrizations,

non-resonant cross sections are accurately described as well. The calculable R matrix is an efficient technique to solve the stationary or time-dependent Schrödinger equation in various situations as well as its relativistic extensions. It underwent most of its developments in atomic physics but we have shown in section 6 that it can also be useful in nuclear physics.

Because of the variety and complexity of its applications, the R -matrix theory has been and is still sometimes misunderstood or misjudged for different reasons. A first often-made criticism concerns the role of the channel radius. The R -matrix formulae depend on this radius which has no strict physical meaning. This criticism cannot be addressed to the calculable R matrix where the independence of the physical results on this radius, provided that it is large enough, is a useful validity test. In the phenomenological R -matrix, however, the channel radius is indeed a parameter whose value is disputable. This arises from the truncation of the R matrix to a small number of poles. In spite of this truncation, this approximation often provides excellent fits to the data. The standard option is to optimize the channel radius together with the other parameters. This radius should however be larger than the sum of the radii of the colliding nuclei. Its value should always be mentioned because the other parameters depend on its choice.

Another criticism deals with a reputation of poor convergence of the calculable R matrix. As we have shown, this reputation is undeserved. Its origin lies in the choice of a common logarithmic derivative for the basis states in the founding papers. While this choice is acceptable (although with some discontinuity drawback) for an infinite basis, it leads to inaccuracies when the basis is truncated. The introduction of the Bloch operator has opened a way to the use of finite bases providing a sufficient variety of behaviours at the boundary for which this problem disappears, a fact not yet known enough. Modern R -matrix codes can employ different types of such bases. They reach an excellent convergence and do not require the use of the Buttle correction.

The calculable R matrix provides bound-state and scattering-state wave functions that can be used in a variety of applications with sometimes technical complications due to the existence of two regions to define the wave function. In atomic, molecular and nuclear physics, the challenge is now to reach the same level of accuracy for processes with more than two unbound particles in the final states. Advances have been made for double ionization by a photon in atomic and molecular physics and for the breakup of two- and three-body halo nuclei in nuclear physics. Progresses of R -matrix theory in these directions should still be expected.

Acknowledgments

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Appendix A. Collision matrix and K matrix

System (2.38) possesses N linearly independent solutions that vanish at the origin. A matrix solution u is obtained by putting those independent solutions as columns of a square matrix. By multiplication on the right by any invertible matrix, one obtains another matrix solution of system (2.38) which is physically equivalent. The most general asymptotic expression of such a matrix generalizes (2.34) as

$$u \xrightarrow{r \rightarrow \infty} v^{-1/2} (I - OU)C, \quad (\text{A1})$$

where U is the collision matrix, I and O are complex conjugate diagonal matrices involving incoming and outgoing Coulomb functions (2.8) on the diagonal and v is a diagonal matrix of velocities. Complex matrix C is arbitrary non-singular. In (2.34), we have chosen C diagonal for simplicity.

With $C = i(1 + U)^{-1}C'$, where matrix C' is also non-singular, an equivalent asymptotic form which is often used is obtained with (2.8) as

$$u \xrightarrow{r \rightarrow \infty} v^{-1/2} (F + GK)C', \quad (\text{A2})$$

where F and G are real diagonal matrices involving regular and irregular Coulomb functions F_l and G_l on the diagonal. This asymptotic form is real if C' is real. It is then the most general asymptotic form of real solutions.

Matrices U and K are related by

$$U = (1 - iK)^{-1} (1 + iK) \quad (\text{A3})$$

or

$$K = i(1 - U)(1 + U)^{-1}. \quad (\text{A4})$$

Matrix K is real and symmetric if U is unitary and symmetric.

Appendix B. Proof of relation (3.27)

Let B be an invertible $N \times N$ matrix and u and v be vectors with N components. The inverse of the square matrix

$$A = B + uv^T \quad (\text{B1})$$

is given by

$$A^{-1} = B^{-1} - \frac{B^{-1}uv^TB^{-1}}{1 + v^TB^{-1}u}, \quad (\text{B2})$$

where the denominator is a scalar. A corollary of (B2) reads

$$A^{-1}u = \frac{B^{-1}u}{1 + v^TB^{-1}u}. \quad (\text{B3})$$

Another corollary is the relation

$$(v^TA^{-1}u)^{-1} = 1 + (v^TB^{-1}u)^{-1} \quad (\text{B4})$$

from which (3.27) follows.

Appendix C. Matrix elements for various basis functions

Here we present the matrix elements used for different basis functions in section 4. Unless specified otherwise the matrix elements of the kinetic energy are given for $l = 0$ and in units of $\hbar^2/2\mu$.

- (i) *Sine functions.* The overlap matrix elements between basis functions (4.3) are given by

$$\langle \varphi_i | \varphi_j \rangle = \frac{a}{2} \delta_{ij}. \quad (\text{C1})$$

The matrix elements for the kinetic energy are simple,

$$\langle \varphi_i | T_0 | \varphi_j \rangle = \frac{\pi^2}{2a} \left(i - \frac{1}{2} \right)^2 \delta_{ij}. \quad (\text{C2})$$

Because of property (4.4) at the boundary, matrix elements of the Bloch operator $\mathcal{L}(0)$ vanish. The matrix elements of $1/r^2$ are also analytical but involve sine integral functions. For the potential, a numerical treatment is necessary.

- (ii) *Gaussian functions.* Let us define

$$\begin{aligned} I_k(v) &= \int_0^a r^k \exp(-v r^2) dr \\ &= \gamma((k+1)/2, va^2)/2v^{(k+1)/2}, \end{aligned} \quad (\text{C3})$$

where γ is the incomplete gamma function and a is implied. The overlap matrix elements between basis functions (4.5) are given by

$$\langle \varphi_i | \varphi_j \rangle = I_{2l+2}(v_i + v_j), \quad (\text{C4})$$

with $v_i = 1/b_i^2$. For the kinetic energy, we have

$$\begin{aligned} \langle \varphi_i | T_l + \mathcal{L}(0) | \varphi_j \rangle &= 4v_i v_j I_{2l+4}(v_i + v_j) \\ &\quad - 2(l+1)(v_i + v_j) I_{2l+2}(v_i + v_j) \\ &\quad + (l+1)(2l+1) I_{2l}(v_i + v_j). \end{aligned} \quad (\text{C5})$$

For a Gaussian potential and for the Coulomb potential, the matrix elements read

$$\langle \varphi_i | \exp(-(r/r_0)^2) | \varphi_j \rangle = I_{2l+2}(v_i + v_j + 1/r_0^2), \quad (\text{C6})$$

$$\langle \varphi_i | 1/r | \varphi_j \rangle = I_{2l+1}(v_i + v_j), \quad (\text{C7})$$

and therefore do not require any numerical integration. Of course, other potentials can be considered, but the matrix elements must be, in general, obtained from a numerical integration.

- (iii) *Lagrange functions.* Let us start with matrix elements in interval $(0, a)$. The regularization coefficient n in (4.7) is taken as $n = 1$. This ensures that the wave function vanishes at the origin and allows that the Coulomb potential is treated accurately at the Gauss approximation. Using wave functions (4.9) and the corresponding Gauss approximation the matrix elements take a very simple form

$$\langle \varphi_i | \varphi_j \rangle = \delta_{ij}, \quad (\text{C8})$$

$$\langle \varphi_i | V | \varphi_j \rangle = V(ax_i) \delta_{ij}, \quad (\text{C9})$$

i.e. they only require the evaluation of the potential at the mesh points. For the kinetic energy, a simple calculation [46] provides for $i = j$

$$\begin{aligned} \langle \varphi_i | T_0 + \mathcal{L}(0) | \varphi_i \rangle \\ = \frac{(4N^2 + 4N + 3)x_i(1 - x_i) - 6x_i + 1}{3a^2x_i^2(1 - x_i)^2} \end{aligned} \quad (\text{C10})$$

and for $i \neq j$,

$$\begin{aligned} \langle \varphi_i | T_0 + \mathcal{L}(0) | \varphi_j \rangle = \frac{(-1)^{i+j}}{a^2[x_ix_j(1 - x_i)(1 - x_j)]^{1/2}} \\ \times \left[N^2 + N + 1 + \frac{x_i + x_j - 2x_ix_j}{(x_i - x_j)^2} \right. \\ \left. - \frac{1}{1 - x_i} - \frac{1}{1 - x_j} \right]. \end{aligned} \quad (\text{C11})$$

Thanks to the Bloch operator, this matrix element is symmetric. For $l \neq 0$, the centrifugal term is included in the potential (C9).

Next we consider (a_1, a_2) intervals which are used in the propagation method. The basis functions (4.7) with $n = 0$ are extended to

$$\begin{aligned} \varphi_i(r) = (-1)^{N+i} (x_i(1 - x_i)\Delta a)^{1/2} \\ \times \frac{P_N((2r - a_1 - a_2)/\Delta a)}{r - x_i\Delta a - a_1}, \end{aligned} \quad (\text{C12})$$

with $\Delta a = a_2 - a_1$, and the Lagrange condition becomes

$$\varphi_i(a_1 + x_j\Delta a) = (\lambda_i\Delta a)^{-1/2}\delta_{ij}. \quad (\text{C13})$$

The matrix elements of the potential read

$$\langle \varphi_i | V | \varphi_j \rangle = V(a_1 + x_i\Delta a)\delta_{ij}, \quad (\text{C14})$$

and are still given by a simple evaluation of the potential at the mesh points. The matrix elements of the kinetic energy are given at the Gauss approximation by

$$\begin{aligned} \langle \varphi_i | T_0 | \varphi_i \rangle = \frac{1}{3\Delta a^2x_i(1 - x_i)} \\ \times \left[N^2 + N + 6 - \frac{2}{x_i(1 - x_i)} \right] \end{aligned} \quad (\text{C15})$$

for $i = j$ and

$$\begin{aligned} \langle \varphi_i | T_0 | \varphi_j \rangle \\ = \frac{(-1)^{i+j}}{\Delta a^2} \sqrt{\frac{x_j(1 - x_j)}{x_i(1 - x_i)}} \frac{2x_ix_j + 3x_i - x_j - 4x_i^2}{x_i(1 - x_i)(x_j - x_i)^2} \end{aligned} \quad (\text{C16})$$

for $i \neq j$. The matrix elements of the Bloch operators read

$$\begin{aligned} \langle \varphi_i | \mathcal{L}_{a_2} | \varphi_j \rangle = \frac{(-1)^{i+j}}{\Delta a^2} \sqrt{\frac{x_ix_j}{(1 - x_i)(1 - x_j)}} \\ \times \left[N(N + 1) - \frac{1}{1 - x_j} \right] \end{aligned} \quad (\text{C17})$$

and

$$\begin{aligned} \langle \varphi_i | \mathcal{L}_{a_1} | \varphi_j \rangle = \frac{(-1)^{i+j}}{\Delta a^2} \sqrt{\frac{(1 - x_i)(1 - x_j)}{x_ix_j}} \\ \times \left[-N(N + 1) + \frac{1}{x_j} \right]. \end{aligned} \quad (\text{C18})$$

Although this does not appear clearly, one can verify that the matrix elements of operator $T_0 + \mathcal{L}_{a_2} - \mathcal{L}_{a_1}$ are symmetric in accord with the fact that this operator is Hermitian over the region (a_1, a_2) .

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