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R-matrix School 2025: Introduction to R-matrix Theory



Marco T. Pigni

May 2025

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Nuclear Energy Fuel Cycle Division

**R-MATRIX SCHOOL 2025:
INTRODUCTION TO R-MATRIX THEORY**

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May 2025

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ABSTRACT

This technical memo serves as lecture material for the R-matrix school 2025 and will be distributed to the participants. The manuscript discusses the introduction to the R-matrix theory in detail, including its algorithm to calculate reaction cross sections and derivations.

1. RESOLVED RESONANCES

Resolved resonances are described most conveniently by the R-matrix theory in its standard form in accordance with the article by Lane and Thomas [1], which provides a comprehensive derivation of the equations. This report defines quantities relevant to the discussion of these lectures using notation similar to that found in Fröhner's report [2]. Additional resources on R-matrix theory can be found in both Larson's SAMMY manual [3] and in the book by Thompson and Nunes, *Nuclear Reactions for Astrophysics* [4], from which these lectures are partly derived.

This report begins with a description of the physical meaning of *neutron-induced resolved resonances*, as shown in Figure 1. The set of cross sections (in this particular case, total cross sections shown in black) feature a rapidly varying resonant behavior which arises from a quasi-bound state of the compound nucleus system, ^{A+1}X , formed by the incident particle (e.g., a neutron) plus a target nucleus, $n+^A\text{X}$. The resonances visible in the total cross sections correspond to the energy levels of the compound nucleus above its neutron separation energy. As the incident neutron energy (and, therefore, the excitation energy of the compound nucleus) increases, a greater number of open channels is available, leading to overlap among several excited states. These concepts can be extended to incident particles other than neutrons such as charged particles, protons, and α -particles.

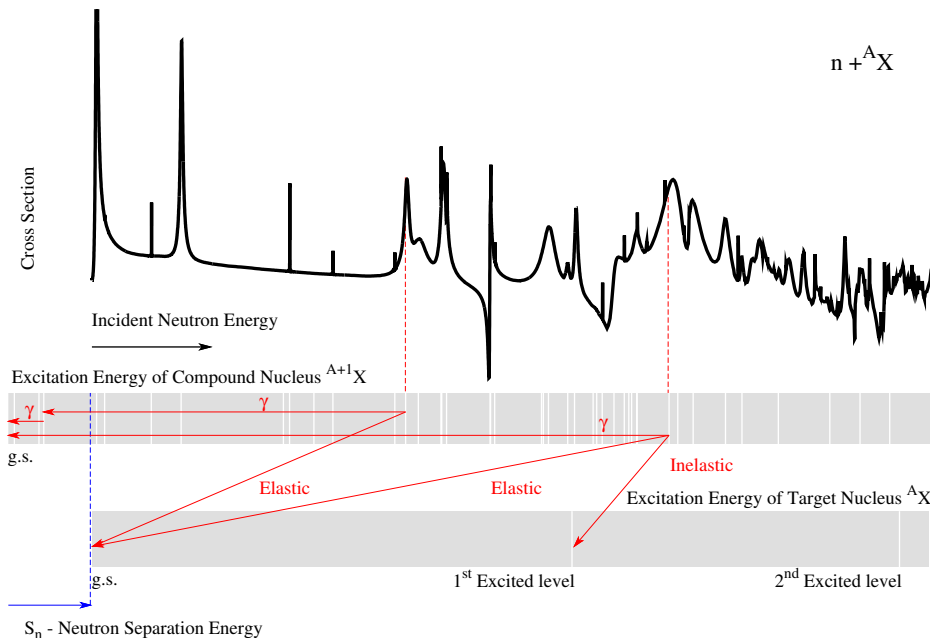


Figure 1. Numerous compound–nucleus resonances of neutron-induced total cross sections are shown in black. The energy spectrum of the formed compound nucleus, ^{A+1}X , corresponds to resonances above its neutron separation energy. As the energy of the incident particle increases, a greater number of open channels is available, thus leading to other reaction channels like inelastic scattering.

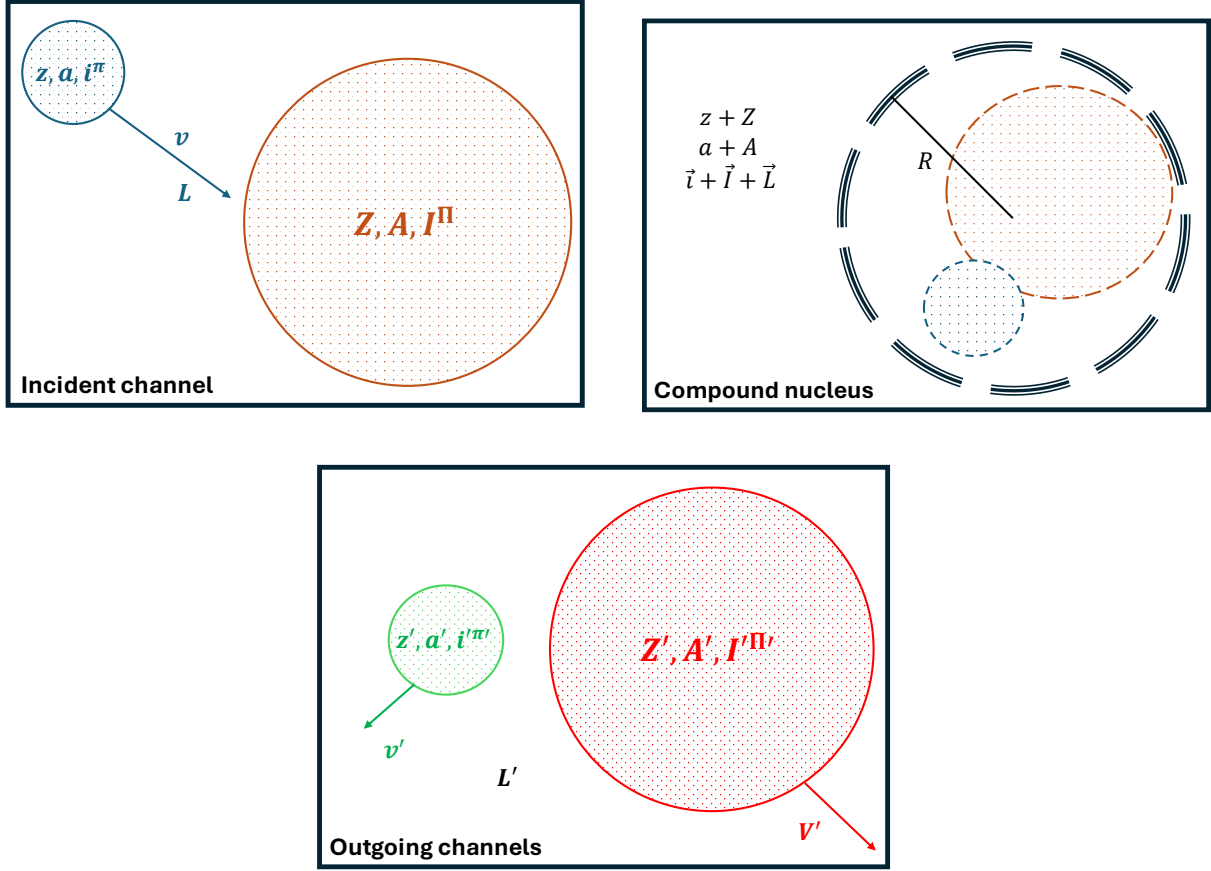


Figure 2. Schematic of incident and outgoing channels in the laboratory system. For the interior region defined within the separation distance R , no assumptions are made about the nature of the interaction. In the figure, z , a , and i^π refer to the charge, mass number, spin and parity of the incident particle with velocity v and related angular momentum l , whereas Z , A , and I^Π refer to the target particle. Primes are used to indicate post-collision quantities.

A *particle pair* or partition is defined as a pair of (incoming or outgoing) particles, including specific information relevant to the interaction of two particles such as their masses and charge numbers, spins, and parities, as schematically shown in Figure 2.

In describing the R -matrix theory formalism, a channel can be conveniently and compactly defined by the label $c = \{\alpha, l, s, J\}$, where

- α represents the (two-body) partition of the compound nucleus system into reaction partners, including their masses (m and M), charge numbers (z and Z), spins (i^π and I^Π) with associated parities, and all other quantum numbers for each of the two particles, as well as the Q -value (in center of mass) or energy threshold (in laboratory system).
- The angular momenta (in units of \hbar) satisfy the quantum mechanical triangle relations:

$$\vec{J} = \vec{l} + \vec{s}, \quad \text{i.e.} \quad |l - s| \leq J \leq l + s,$$

$$\vec{s} = \vec{i} + \vec{I}, \quad \text{i.e.} \quad |I - i| \leq s \leq I + i,$$

where, omitting the superscripts for the parity,

l is the orbital angular momentum of the pair with associated parity given by $(-1)^l$,

s represents the channel spin (and associated parity) of the vector sum of the spins of the particle-pair defined by the quantity α , $\vec{s} = \vec{i} + \vec{I}$, and

J is the total angular momentum (and associated parity) of the vector sum of angular momentum l and channel spin s , $\vec{J} = \vec{l} + \vec{s}$.

Only J and the associated parity are conserved for any given interaction. The other quantum numbers may differ from channel to channel as long as the sum rules for spin and parity are obeyed. The set of all channels with the same J and π are called a *spin group*.

The angle-integrated reaction cross section $\sigma_{cc'}$, calculated from the incident c and exit channel c' with a total angular momentum J , can be written in terms of the scattering matrix $U_{cc'}^J$, as

$$\sigma_{cc'} = \frac{\pi}{k_c^2} g_J |e^{+2iw_c} \delta_{cc'} - U_{cc'}^J|^2 \delta_{JJ'}, \quad (1)$$

where the wave number associated with the incident particle pair $\alpha \equiv \alpha_c$ in the center of mass of the incident channel c having incident (moving) particle of mass m and laboratory kinetic energy E is

$$k_c = \frac{1}{\hbar} \frac{M}{(m+M)} \sqrt{2mE}. \quad (2)$$

The spin statistical factor for given spins i and I of the two collision partners for the channel c is

$$g_J = \frac{2J+1}{(2i+1)(2I+1)}, \quad (3)$$

and the quantity w_c is the Coulomb phase-shift difference that is zero for non-Coulomb channels. The scattering matrix U can be written in terms of matrix W as

$$U_{cc'} = \Omega_c W_{cc'} \Omega_{c'}, \quad (4)$$

where Ω_c is given by

$$\Omega_c = e^{i(w_c - \varphi_c)}, \quad (5)$$

as defined by w_c and the potential scattering phase shifts that are reported in Table 1 for non-Coulomb interactions. In matrix notation with indices suppressed, the matrix W in Eq. (4) is related to the R matrix via the relation

$$W = P^{\frac{1}{2}} (\mathbb{I} - \mathbf{R}L)^{-1} (\mathbb{I} - \mathbf{R}L^*) P^{-\frac{1}{2}}, \quad (6)$$

where quantities in bold denote non-diagonal matrices. The quantity \mathbb{I} represents the identity matrix, and superscript $*$ indicates a complex conjugate. The quantity L in Eq. (6) is given by

$$L = (S - B) + iP, \quad (7)$$

with P being the penetration factor (penetrability), S the shift factor, and B the arbitrary boundary constant calculated at the channel radius a_c . P and S are functions of energy E depending on the orbital angular momentum l and the channel radius a_c .

Although Eq. (6) is correct, the following equivalent form is used to compute the reaction cross sections as numerically more stable,

$$\begin{aligned}
\mathbf{W} &= P^{\frac{1}{2}}(\mathbb{I} - \mathbf{R}L)^{-1}(\mathbb{I} - \mathbf{R}L^*)P^{-\frac{1}{2}} \\
&= P^{\frac{1}{2}}(\mathbb{I} - \mathbf{R}L)^{-1}(I - \mathbf{R}L + 2i\mathbf{R}P)P^{-\frac{1}{2}} \\
&= P^{\frac{1}{2}}[(\mathbb{I} - \mathbf{R}L)^{-1}(\mathbb{I} - \mathbf{R}L) + 2i(\mathbb{I} - \mathbf{R}L)^{-1}\mathbf{R}P]P^{-\frac{1}{2}} \\
&= P^{\frac{1}{2}}P^{-\frac{1}{2}} + 2iP^{\frac{1}{2}}(\mathbb{I} - \mathbf{R}L)^{-1}\mathbf{R}PP^{-\frac{1}{2}} \\
&= \mathbb{I} + 2iP^{\frac{1}{2}}(\mathbb{I} - \mathbf{R}L)^{-1}\mathbf{R}P^{\frac{1}{2}} \\
&= \mathbb{I} + 2iP^{\frac{1}{2}}L^{-1}(L^{-1} - \mathbf{R})^{-1}\mathbf{R}P^{\frac{1}{2}},
\end{aligned} \tag{8}$$

where the non-diagonal matrix \mathbf{X} in its index form becomes

$$X_{cc'} = P_c^{\frac{1}{2}}L_c^{-1} \sum_{c''} \left[(L^{-1} - \mathbf{R})^{-1} \right]_{cc''} \mathbf{R}_{c''c'} P_{c'}^{\frac{1}{2}} \delta_{JJ'} \tag{9}$$

The penetrability $P_c \rightarrow P_l(\rho, \eta)$ and shift factors $S_c \rightarrow S_l(\rho, \eta)$ have their most general form in terms of the regular and irregular Coulomb functions $F_l \equiv F_l(\rho, \eta)$ and $G_l \equiv G_l(\rho, \eta)$, respectively, as

$$P_l = \frac{\rho}{F_l^2 + G_l^2} \quad \text{and} \quad S_l = \rho \frac{\dot{F}F + \dot{G}G}{F_l^2 + G_l^2}, \tag{10}$$

where the overscript dot refers to partial derivatives with respect to ρ . This is related to the center-of-mass momentum which, in turn, is related to the wave number depending from the laboratory energy of the incident particle E . For an arbitrary channel c with particle pair α , orbital angular momentum l , and channel radius a_c , ρ has the form

$$\rho = k_\alpha a_c = \frac{1}{\hbar} \sqrt{2\mu_\alpha \frac{M}{m+M}} \sqrt{(E - \Xi_\alpha)} a_c. \tag{11}$$

The quantity Ξ_α is the energy threshold for the particle pair α , and m and M are the masses of the incident particle and target nucleus, respectively, in the laboratory frame of reference. In Eq. (10), η is the energy-dependent Sommerfeld parameter that is given by

$$\eta_\alpha = \frac{z_\alpha Z_\alpha e^2 \mu_\alpha}{\hbar^2 k_\alpha}, \tag{12}$$

where $\mu_\alpha = m_\alpha M_\alpha / (m_\alpha + M_\alpha)$ is the reduced mass defined by the masses of the particle-pair α .

In the particular case of neutron-induced reaction, in which the Sommerfeld parameter is zero, appropriate formulae¹ for P , S , and φ are reported in Table 1.

Formulae for a particular cross-section type can be derived by summing over the terms in Eq. (1). For the

¹To avoid ambiguity, it should be stated that below the channel threshold, that is, for $(E - \Xi_\alpha) < 0$, SAMMY uses the convention of Lane-Thomas, namely setting $P_c = 0$ and $S_c = \text{Re}(L_c) = L_c$ instead of using an analytical continuation of the shift and penetrability function in the complex plane by computing the expressions in Table 1 as a function of an imaginary ρ for which $iP_c(\rho)$ becomes real-valued but separate from $S_c(\rho)$.

Table 1. Hard-sphere penetrability (penetration factor) P , level shift factor S , and potential-scattering phase shift φ for orbital angular momentum l , wave number k , and channel radius a_c , with $\rho = ka_c$

l	P_l	S_l	φ_l
0	ρ	0	ρ
1	$\rho^3/(1+\rho^2)$	$-1/(1+\rho^2)$	$\rho - \tan^{-1} \rho$
2	$\rho^5/(9+3\rho^2+\rho^4)$	$-(18+3\rho^2)/(9+3\rho^2+\rho^4)$	$\rho - \tan^{-1} [3\rho/(3-\rho^2)]$
\vdots	\vdots	\vdots	\vdots
l	$\frac{\rho^2 P_{l-1}}{(1-S_{l-1})^2 + P_{l-1}^2}$	$\frac{\rho^2(l-S_{l-1})}{(1-S_{l-1})^2 + P_{l-1}^2} - l$	$\varphi_{l-1} - \tan^{-1} (P_{l-1}/(l-S_{l-1}))^\dagger$

[†] The iterative formula for φ_l could also be defined by $B_l = (B_{l-1} + X_l)/(1 - B_{l-1}X_l)$, where $B_l = \tan(\rho - \varphi_l)$ and $X_l = P_{l-1}/(l - S_{l-1})$.

total cross section, the sum over all possible exit channels and all spin groups gives

$$\begin{aligned}
 \sigma_{\text{tot}} &= \sum_c \sum_{c'} \sum_J \frac{\pi}{k_c^2} g_J |\delta_{cc'} - U_{cc'}|^2 \\
 &= \frac{\pi}{k_c^2} \sum_J g_J \sum_c \sum_{c'} \left(\delta_{cc'} - U_{cc'} \delta_{cc'} - U_{cc'}^* \delta_{cc'} + |U_{cc'}|^2 \right) \\
 &= \frac{2\pi}{k_c^2} \sum_J g_J \sum_c \left[1 - \text{Re}\{U_{cc}\} \right].
 \end{aligned} \tag{13}$$

For neutral or non-charged incident particles, the elastic (or scattering) cross section $c = c'$ is given by

$$\sigma_{\text{ela}} = \frac{\pi}{k_c^2} \sum_J g_J \sum_{c=\text{incident channel}} \left[1 - 2 \text{Re}\{U_{cc}\} + \sum_{c'=\text{incident channel}} |U_{cc'}|^2 \right]. \tag{14}$$

Similarly, the cross section for any non-elastic reaction can be written as

$$\sigma_{\text{rea}} = \frac{\pi}{k_c^2} \sum_J g_J \sum_{c=\text{incident channel}} \sum_{c'=\text{reaction channel}} |U_{cc'}|^2. \tag{15}$$

In particular, the capture cross section could be written as the difference between the total and all other cross sections,

$$\sigma_{\text{cap}} = \frac{\pi}{k_c^2} \sum_J g_J \sum_{c=\text{incident channel}} \left(1 - \sum_{c'=\text{all channels except capture}} |U_{cc'}|^2 \right). \tag{16}$$

1.1 R-MATRIX AND A-MATRIX EQUATIONS

The **R** matrix introduced in Eq. (6) is defined by the energy-dependent R-matrix function in its general form as

$$\mathbf{R}_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_\lambda - E} \delta_{J,J'}, \tag{17}$$

where E_λ represents the energy for the resonance level λ with reduced width-amplitude γ related to the partial width Γ by

$$\Gamma_{\lambda c} = 2P_c \gamma_{\lambda c}^2. \quad (18)$$

Note that in Eq. (17), the energies and widths are given in laboratory frame of reference. The summation in Eq. (17) contains an infinite number of levels. All channels, including the “gamma channel” for which one of the particles is a photon, are represented by the channel indices.

The scattering matrix can be parameterized not only by the \mathbf{R} matrix (expressed in terms of channel–channel interactions), but also by the level matrix \mathbf{A} that is expressed in terms of level–level interactions:

$$A_{\mu\lambda}^{-1} = (E_\lambda - E) \delta_{\mu\lambda} - \sum_c \gamma_{\mu c} L_c \gamma_{\lambda c}. \quad (19)$$

To see the relationship of the \mathbf{A} matrix to the \mathbf{R} matrix, the first step is to multiply both sides of Eq. (19) by \mathbf{A} and sum over the level index λ ,

$$\begin{aligned} \sum_\lambda A_{\mu\lambda}^{-1} A_{\lambda\nu} &= \sum_\lambda (E_\lambda - E) \delta_{\mu\lambda} A_{\lambda\nu} - \sum_c \gamma_{\mu c} L_c \gamma_{\lambda c} A_{\lambda\nu}, \\ &\Downarrow \\ \delta_{\mu\nu} &= (E_\mu - E) A_{\mu\nu} - \sum_c \gamma_{\mu c} L_c \sum_\lambda \gamma_{\lambda c} A_{\lambda\nu}. \end{aligned} \quad (20)$$

Dividing by $(E_\mu - E)$, multiplying on the left by $\gamma_{\mu c'}$ and on the right by $\gamma_{\nu c''}$, and summing over μ , the form of the equation becomes

$$\begin{aligned} \sum_\mu \gamma_{\mu c'} (E_\mu - E)^{-1} \delta_{\mu\nu} \gamma_{\nu c''} &= \sum_\mu \gamma_{\mu c'} (E_\mu - E)^{-1} (E_\mu - E) A_{\mu\nu} \gamma_{\nu c''} \\ &\quad - \sum_\mu \gamma_{\mu c'} (E_\mu - E)^{-1} \sum_c \gamma_{\mu c} L_c \sum_\lambda \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}, \end{aligned} \quad (21)$$

which can be reduced to

$$\begin{aligned} \gamma_{\nu c'} (E_\nu - E)^{-1} \gamma_{\nu c''} &= \sum_\mu \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} \\ &\quad - \sum_c \left[\sum_\mu \gamma_{\mu c'} (E_\mu - E)^{-1} \gamma_{\mu c} \right] L_c \sum_\lambda \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}. \end{aligned} \quad (22)$$

Summing over ν puts this into the form

$$\begin{aligned} \left[\sum_\nu \gamma_{\nu c'} (E_\nu - E)^{-1} \gamma_{\nu c''} \right] &= \sum_{\mu\nu} \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} \\ &\quad - \sum_c \left[\sum_\mu \gamma_{\mu c'} (E_\mu - E)^{-1} \gamma_{\mu c} \right] L_c \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}, \end{aligned} \quad (23)$$

in which the quantities in square brackets can be replaced with the \mathbf{R} matrix, giving

$$\begin{aligned}
\mathbf{R}_{c'c''} &= \sum_{\mu\nu} \gamma_{\mu c'} \mathbf{A}_{\mu\nu} \gamma_{\nu c''} - \sum_c \mathbf{R}_{c'c} L_c \sum_{\lambda\nu} \gamma_{\lambda c} \mathbf{A}_{\lambda\nu} \gamma_{\nu c''}, \\
&= \sum_c [\delta_{c'c} - \mathbf{R}_{c'c} L_c] \sum_{\lambda\nu} \gamma_{\lambda c} \mathbf{A}_{\lambda\nu} \gamma_{\nu c''}.
\end{aligned} \tag{24}$$

Solving for the summation, this equation can be rewritten as

$$[(\mathbb{I} - \mathbf{R}\mathbf{L})^{-1} \mathbf{R}]_{cc''} = \sum_{\lambda\nu} \gamma_{\lambda c} \mathbf{A}_{\lambda\nu} \gamma_{\nu c''}. \tag{25}$$

Comparing Eq. (25) to Eq. (8) gives, in matrix notation,

$$\mathbf{W} = \mathbb{I} + 2iP^{\frac{1}{2}} \boldsymbol{\gamma}^\top \mathbf{A} \boldsymbol{\gamma} P^{\frac{1}{2}}. \tag{26}$$

These equations are exact because no approximations have been made.

1.2 REICH-MOORE APPROXIMATION

One approximation commonly made for RRR evaluation of nuclei with a large number of capture channels is to “eliminate” them by treating them in aggregate, since individual capture channel cross sections are ordinarily not measured. This is the Reich–Moore (RM) approximation in which the total capture cross section is parameterized by adding an imaginary (total) capture width to the resonance energy appearing inside the R-matrix, and the capture cross section is calculated as a deviation from unitarity of the approximate R-matrix. The approximation is most clearly explained via the definition A-matrix Eq. (19); neglecting the off-diagonal for the photon channels, this equation can be approximated as

$$\mathbf{A}_{\mu\lambda}^{-1} \approx (E_\lambda - E) \delta_{\mu\lambda} - \left[\sum_{\substack{c=\text{photon} \\ \text{channels}}} \gamma_{\mu\gamma} L_\gamma \gamma_{\lambda\gamma} \right] \delta_{\mu\lambda} - \sum_{\substack{c=\text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}. \tag{27}$$

The off-diagonal elements of the matrix in square brackets have been assumed to be negligible relative to the diagonal and approximated by zero, due to cancellations among the terms summed over in the expression for off-diagonal elements. The accuracy of this approximation increases with increasing number of capture channels, increasing randomness of signs of capture partial width amplitudes (PWAs), and decreasing correlations among the capture PWAs between different levels². For gamma channels $c \in \gamma$, the quantity $L = S - B + iP$ reduces to $L_\gamma = S_\gamma - B_\gamma + i$, and Eq. (27) becomes

$$\mathbf{A}_{\mu\lambda}^{-1} \approx (E_\lambda + \Delta_{\lambda\gamma} - E - i\bar{\Gamma}_{\lambda\gamma}/2) \delta_{\mu\lambda} - \sum_{\substack{c=\text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}, \tag{28}$$

where the level shift for the photon channel $\Delta_{\lambda\gamma}$ is usually absorbed in the resonance energy E_λ . The bar over $\bar{\Gamma}_{\lambda\gamma}$ is used to indicate that the RM width is the sum of all possible gamma transitions within the photon channel.

In this form, the expression for the matrix \mathbf{A} is analogous to the exact expression in Eq. (19) with two modifications: the additional imaginary term is added to the energy difference, and the sum over the channels includes only the particle channels (non-eliminated channels). It is therefore possible to immediately write the R-matrix formula for the eliminated-channel approximation as

²Fulfillment of these conditions is known as random phase hypothesis.

$$\mathbf{R}_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda\gamma}/2} \delta_{JJ'}, \quad (29)$$

where the channel indices c and c' refer only to particle channels, not to the gamma channels. This \mathbf{R} matrix formula is the RM approximation and is the form used in the SAMMY code.

1.3 THE PRACTICALLY IMPORTANT A-MATRIX APPROXIMATIONS

The practically important approximations of the R-matrix theory can be easily described in the inverse of the level matrix \mathbf{A} in the following convenient manner. Recalling the quantity $L_c = (B_c - S_c) + iP_c$, one has

- **Wigner–Eisenbud representation** (exact)

With boundary condition $B_c \in \mathbb{R}$ and constant, e.g. $B_c = -I_c$:

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_{\lambda} - E) \delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} L_c \gamma_{\mu c}.$$

The eigenvalues E_{λ} and decay amplitudes $\gamma_{\lambda c}$ are real and constant. Unitarity of the scattering matrix is implicitly preserved.

- **Reich–Moore approximation (RM)**

Off-diagonal contributions of the photon channels $c \in \gamma$ are neglected:

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_{\lambda} + \Delta_{\lambda\gamma} - E - i\bar{\Gamma}_{\lambda\gamma}/2) \delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} L_c \gamma_{\mu c}.$$

The eigenvalues E_{λ} and decay amplitudes $\gamma_{\lambda c}$ are real and constant, as well as the gamma radiation width: $\bar{\Gamma}_{\lambda\gamma} = \sum_{c \in \gamma} \Gamma_{\lambda c}$. The scattering matrix is not unitary, but the unitarity on the scattering matrix is assumed in calculating the capture cross section, as shown for neutral particle in Eq. (16).

- **Kapur–Peierls representation** (exact)

With the complex boundary $B_c = S_c + iP_c$, one has $L_c = 0$:

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_{\lambda} - E) \delta_{\lambda\mu}.$$

The eigenvalues E_{λ} and decay amplitudes $\gamma_{\lambda c}$ are complex, with implicit energy dependence. This boundary condition removes the need for matrix inversion because $(\mathbb{I} - \mathbf{RL}) = \mathbb{I}$, but this leads to complex, energy-dependent resonance parameters.

- **Single-level Breit–Wigner approximation (SLBW)**

Only one level retained $\lambda = k$, and all others neglected:

$$\mathbf{A}^{-1} = (E_k - E) - \sum_c L_c \gamma_{kc}^2 = E_k + \Delta_k - E - i\Gamma_k.$$

Level shift Δ_k and total with $\Gamma_k = \sum_c \Gamma_c$ real with explicit energy dependencies.

- **Multi-level Breit–Wigner approximation (MLBW)**

Off-diagonal elements of the inverse of the level matrix \mathbf{A}^{-1} neglected

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_{\lambda} - E - \sum_c \gamma_{\lambda c}^2 L_c) \delta_{\lambda\mu} = (E_{\lambda} + \Delta_{\lambda} - E - i\Gamma_{\lambda}/2) \delta_{\lambda\mu}.$$

Level shift Δ_k and total with $\Gamma_k = \sum_c \Gamma_c$ real with explicit energy dependencies.

- **Adler–Adler approximation (AA)**

The quantity L_c is calculated at the corresponding resonance energy E_λ (E_μ), neglecting its energy dependence:

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_\lambda - E) \delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} \sqrt{L_c(E_\lambda)L_c(E_\mu)} \gamma_{\mu c}.$$

1.4 DERIVATION OF SCATTERING THEORY EQUATIONS

In previous sections, the scattering matrix \mathbf{U} for the incident particle energy E_{lab} was written in terms of the \mathbf{R} matrix via the matrices \mathbf{W} , Ω , L , and P , depending on a set of resonance parameters. However, the relation between \mathbf{U} and \mathbf{R} matrices was presented without discussing the form of the R-matrix function of Eq. (17) and neglecting the role of the set of resonance parameters in that derivation. In this section, a brief derivation of the R-matrix function is discussed.

It is first assumed that it is possible to define a region above a distance R (in radial coordinates) if the nuclear forces are negligible. The distance a (usually in units of Fermi or fm) allows for definition of the radial wave functions $u \equiv u(R)$ in the external ($R > a$) and internal ($R < a$) region, matching at the distance $R = a$ and forming the total wave function $\psi \equiv \psi(R, \cos(\theta))$ at any radial and angular distance and at general energy E defined in the center of mass of two nuclei.

1.4.1 Schrödinger Equation

Limiting the discussion to the case of elastic scattering of spinless particles³, the Hamiltonian H with a complex potential having a real and an imaginary component, V and W , respectively, is

$$H\psi = (T + V + iW)\psi = E\psi, \quad (30)$$

where, following the partial expansion of the wave function ψ with the Legendre Polynomial $P_l \equiv P_l(\cos(\theta))$ for each partial wave l ,

$$\psi(R, \cos(\theta)) = \sum_{l=0}^{\infty} \frac{u_l(R)}{R} P_l(\cos(\theta)). \quad (31)$$

The kinetic operator T in radial coordinates is

$$T = -\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dR^2} - \frac{l(l+1)}{R^2} \right], \quad (32)$$

with reduced mass μ , and the conditions on the wave function are that $|\psi|^2$ is everywhere finite and that $u_l(R) = 0$ for $R = 0$.

1.4.2 Solutions in the External Region

In the external region $R > a$, the nuclear forces are zero ($V = W = 0$), reducing the Hamiltonian to

$$\frac{d^2 u_l}{dR^2} + \left[k^2 - \frac{l(l+1)}{R^2} \right] u_l = 0, \quad (33)$$

with $k^2 = 2\mu E/\hbar^2$, and therefore having solutions of the following form:

$$u_l(R) = I_l(R) - U_l O_l(R). \quad (34)$$

³For a more general discussion see Section VII.1 of [1]

$I_l \equiv I_l(kR, \eta)$ and $O_l \equiv O_l(kR, \eta)$ represent an incoming and outgoing free wave, respectively, with η being the Sommerfeld Coulomb parameter. U_l is the *collision function* or *S function* that describes the effects of the nuclear interaction, giving both the attenuation and the phase shift of the outgoing wave as

$$\begin{aligned} |U_l|^2 &= 1 \text{ for } W = 0, \\ |U_l|^2 &< 1 \text{ for } W \neq 0, \end{aligned} \quad (35)$$

and the goal is to determine an appropriate analytic form for U_l .

1.4.3 Orthogonal Eigenvectors in Interior Region

For the interior region $R < a$, one starts to define a set of eigenfunctions $w_{\lambda l} \equiv w_{\lambda l}(R)$ and eigenvalues E_λ for a real potential ($V \in \mathbb{R}$ and $W = 0$), satisfying

$$\frac{d^2 w_{\lambda l}}{dR^2} + \left[k_\lambda^2 - \frac{2\mu}{\hbar^2} V - \frac{l(l+1)}{R^2} \right] w_{\lambda l} = 0, \quad (36)$$

with eigenvalues (in center of mass reference)

$$E_\lambda = \frac{\hbar^2 k_\lambda^2}{2\mu}. \quad (37)$$

To ensure that the set of eigenfunctions of Eq. (36) are orthogonal, $w_{\lambda l}$ must satisfy the boundary condition $w_{\lambda l}(R) = 0$ for $R = 0$, together with its logarithmic derivative with respect to R calculated at the distance $R = a$ fixed at some constant value B_l as

$$a \frac{w'_{\lambda l}(a)}{w_{\lambda l}(a)} = B_l. \quad (38)$$

Note that $w_{\lambda l}(R) \in \mathbb{R}$ if the boundary parameter B_l is chosen to be real. The set of eigenfunctions defined with the two conditions above is orthogonal, and this can be demonstrated by

$$\begin{aligned} \int_{R=0}^{R=a} \left(\frac{d^2 w_{\lambda l}}{dR^2} w_{\nu l} - w_{\lambda l} \frac{d^2 w_{\nu l}}{dR^2} \right) dR &= \int_{R=0}^{R=a} \frac{d}{dR} \left(\frac{dw_{\lambda l}}{dR} w_{\nu l} - w_{\lambda l} \frac{dw_{\nu l}}{dR} \right) dR \\ &= \left[\frac{dw_{\lambda l}}{dR} w_{\nu l} - w_{\lambda l} \frac{dw_{\nu l}}{dR} \right]_{R=0}^{R=a} \\ &= \frac{dw_{\lambda l}}{dR} \Big|_{R=a} w_{\nu l}(a) - w_{\lambda l}(a) \frac{dw_{\nu l}}{dR} \Big|_{R=a} \\ &= \frac{B_l}{a} \left(w_{\lambda l}(a) w_{\nu l}(a) - w_{\lambda l}(a) w_{\nu l}(a) \right) = 0, \end{aligned} \quad (39)$$

in which the conditions at the origin on each eigenfunction, $w_{\lambda l}(R) = 0$ for $R = 0$, and Eq. (38), have in fact been invoked. The logarithmic condition on the eigenfunction is the additional condition or *R-matrix trick* used to ensure the wave function orthogonality over a finite range $[0, a]$. Similarly, the integral in Eq. (39) can be evaluated using Eq. (36), giving

$$\begin{aligned} \int_{R=0}^{R=a} \left(\frac{d^2 w_{\lambda l}}{dR^2} w_{\nu l} - w_{\lambda l} \frac{d^2 w_{\nu l}}{dR^2} \right) dR &= \int_{R=0}^{R=a} \left[\left(-k_\lambda^2 - \frac{2\mu V}{\hbar^2} \right) w_{\lambda l} w_{\nu l} - w_{\lambda l} \left(-k_\nu^2 - \frac{2\mu V}{\hbar^2} \right) w_{\nu l} \right] dR \\ &= \int_{R=0}^{R=a} \left(-k_\lambda^2 w_{\lambda l} w_{\nu l} + k_\nu^2 w_{\lambda l} w_{\nu l} \right) dR \\ &= -(k_\lambda^2 - k_\nu^2) \int_{R=0}^{R=a} w_{\lambda l} w_{\nu l} dR. \end{aligned} \quad (40)$$

Equating Eq. (39) to Eq. (40) gives

$$(k_\lambda^2 - k_\nu^2) \int_{R=0}^{R=a} w_{\lambda l} w_{\nu l} dR = 0. \quad (41)$$

For $\lambda \neq \nu$, assuming no degenerate states, it therefore follows that

$$\int_{R=0}^{R=a} w_{\lambda l} w_{\nu l} dR = 0 \quad \text{if } \lambda \neq \nu. \quad (42)$$

The orthogonality of the eigenvectors is therefore established. It is assumed that these wave functions are normalized such that

$$\int_{R=0}^{R=a} w_{\lambda l} w_{\nu l} dR = \delta_{\lambda\nu}. \quad (43)$$

1.4.4 Matching at the Surface

The next step is to define the internal wave function for the Hamiltonian, also including the complex component W of the potential. As basis states, the strategy uses the eigenfunctions found for the real component V and expanded as

$$u_l(R) = \sum_{\lambda} c_{\lambda l} w_{\lambda l}(R) \quad \text{for } R \leq a, \quad (44)$$

with coefficients (to be determined) given by

$$c_{\lambda l} = \int_{R=0}^{R=a} u_l w_{\lambda l} dR \quad (45)$$

and found by multiplying Eq. (44) by $u_{\lambda l}(R)$, integrating over the interval $[0, a]$, and applying the orthogonality relation of Eq. (43).

Starting by considering the integral

$$\int_{R=0}^{R=a} \left(u_l'' w_{\lambda l} - u_l w_{\lambda l}'' \right) dR = \int_{R=0}^{R=a} \left(\frac{d^2 u_l}{dR^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dR^2} \right) dR, \quad (46)$$

this can be expanded by the use of Eqs. (30) and (36) to give

$$\begin{aligned} & \int_{R=0}^{R=a} \left(\frac{d^2 u_l}{dR^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dR^2} \right) dR \\ &= \int_{R=0}^{R=a} \left\{ \left[k^2 - \frac{2\mu}{\hbar^2} (V + iW) - \frac{l(l+1)}{R^2} \right] u_l w_{\lambda l} + u_l \left[k_\lambda^2 - \frac{2\mu}{\hbar^2} V - \frac{l(l+1)}{R^2} \right] w_{\lambda l} \right\} dR \\ &= (k_\lambda^2 - k^2) \int_{R=0}^{R=a} u_l w_{\lambda l} dR + \frac{2\mu}{\hbar} \int_{R=0}^{R=a} W u_l w_{\lambda l} dR. \end{aligned} \quad (47)$$

Defining $\overline{W}_{\lambda l}$ as

$$\overline{W}_{\lambda l} = \frac{\int_{R=0}^{R=a} W u_l w_{\lambda l} dR}{\int_{R=0}^{R=a} u_l w_{\lambda l} dR} \quad (48)$$

allows Eq. (47) to be rewritten in the form

$$\int_{R=0}^{R=a} \left(\frac{d^2 u_l}{dR^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dR^2} \right) dR = \left(k_\lambda^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) \int_{R=0}^{R=a} u_l w_{\lambda l} dR. \quad (49)$$

Integrating the left-hand side of this equation gives

$$\begin{aligned} \int_{R=0}^{R=a} \left(\frac{d^2 u_l}{dR^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dR^2} \right) dR &= \left[\frac{du_l}{dR} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dR} \right]_{R=0}^{R=a} = \left[\frac{du_l}{dR} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dR} \right]_{R=a} \\ &= \left[\frac{du_l}{dR} w_{\lambda l} - u_l \frac{B_l}{a} w_{\lambda l} \right]_{R=a} = \left[a \frac{du_l}{dR} - u_l B_l \right]_{R=a} \frac{w_{\lambda l}(a)}{a}, \end{aligned} \quad (50)$$

in the boundary condition of Eq. (38) which has again been used. Integrating the right-hand side of Eq. (49) by applying Eq. (45) gives

$$\left(k_\lambda^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) \int_{R=0}^{R=a} u_l w_{\lambda l} dR = \left(k_\lambda^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) c_{\lambda l}. \quad (51)$$

Equating Eqs. (50) and (51), therefore, gives

$$\left[a \frac{du_l}{dR} - u_l B_l \right]_{R=a} \frac{w_{\lambda l}}{a} = \left(k_\lambda^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) c_{\lambda l} = \frac{2\mu}{\hbar^2} (E_\lambda - E + i \overline{W}_{\lambda l}) c_{\lambda l}, \quad (52)$$

or, solving for the coefficients $c_{\lambda l}$,

$$c_{\lambda l} = \frac{\hbar^2 w_{\lambda l}(a)}{2\mu a (E_\lambda - E - i \overline{W}_{\lambda l})} \left[a \frac{du_l}{dR} - u_l B_l \right]_{R=a}. \quad (53)$$

Inserting this into Eq. (44) gives

$$u_l(r) = \sum_{\lambda} w_{\lambda l}(r) \frac{\hbar^2 w_{\lambda l}(a)}{2\mu a (E_\lambda - E - i \overline{W}_{\lambda l})} \left[a \frac{du_l}{dr} - u_l B_l \right]_{R=a}, \quad (54)$$

which, when evaluated at $R = a$, becomes

$$u_l(a) = \sum_{\lambda} \frac{\hbar^2 w_{\lambda l}^2(a)}{2\mu a (E_\lambda - E - i \overline{W}_{\lambda l})} \left[a \frac{du_l}{dr} - u_l B_l \right]_{R=a}. \quad (55)$$

Rearranging, this becomes

$$\begin{aligned} u_l(a) &= \left[a \frac{du_l}{dR} - u_l B_l \right]_{R=a} \sum_{\lambda} \frac{\hbar^2 w_{\lambda l}^2(a)/2\mu a}{(E_\lambda - E - i \overline{W}_{\lambda l})} \\ &= \left[a u_l' - u_l B_l \right]_{R=a} \sum_{\lambda} \frac{\gamma_{\lambda l}^2}{(E_\lambda - E - i \overline{\Gamma}_{\lambda l}/2)}, \end{aligned} \quad (56)$$

in which the decay amplitude $\gamma_{\lambda l}$ is defined as

$$\gamma_{\lambda l} \equiv \sqrt{\frac{\hbar^2 w_{\lambda l}^2(a)}{2\mu a}} \quad (57)$$

and the absorption width $\Gamma_{\lambda l}$ is defined as

$$\Gamma_{\lambda l} \equiv 2\overline{W}_{\lambda l}. \quad (58)$$

If the R-function (in the center of mass) is then defined as

$$\mathbf{R}_l = \sum_{\lambda} \frac{\gamma_{\lambda l}^2}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda l}/2}, \quad (59)$$

then Eq. (56) can be written in the form

$$u_l = \left[a u'_l(a) - u_l(a) B_l \right] \mathbf{R}_l, \quad (60)$$

in which everything is evaluated at the matching radius a . Note that the form of Eq. (59) (which is in the CoM frame) is the same as if it were in the laboratory frame of reference. This is because of canceling terms in the numerator and denominator of the R-matrix, as in

$$\begin{aligned} E &\equiv E^{(\text{lab})} = \frac{M}{m+M} E^{(\text{CoM})}, \\ E_{\lambda} &\equiv E_{\lambda}^{(\text{lab})} = \frac{M}{m+M} E_{\lambda}^{(\text{CoM})}, \\ \gamma_{\lambda,l}^2 &\equiv (\gamma_{\lambda,l}^{(\text{lab})})^2 = \frac{M}{m+M} (\gamma_{\lambda,l}^{(\text{CoM})})^2, \text{ and} \\ \Gamma_{\gamma,l} &\equiv \Gamma_{\gamma,l}^{(\text{lab})} = \frac{M}{m+M} \Gamma_{\gamma,l}^{(\text{CoM})}. \end{aligned} \quad (61)$$

Because of this relationship, Eq. (59) can be used for center of mass or laboratory frame parameters. Conventional SAMMY parameterization is to use the laboratory frame.

1.4.5 Spinless particle Scattering Matrix in Terms of R-matrix

Equation (60) for spinless⁴ particles can be converted into the usual R-matrix formulae by inserting Eq. (34),

$$u_l = I_l - U_l O_l, \quad (62)$$

yielding

$$I_l - U_l O_l = \left[a (I'_l - U_l O'_l) - B_l (I_l - U_l O_l) \right] \mathbf{R}_l, \quad (63)$$

in which the primes are related to the partial derivatives with respect to the radial coordinate R , and all quantities are evaluated at the matching radius a . Solving Eq. (63) for U gives

$$U_l \left[-O_l + \mathbf{R}_l (a O'_l - B_l O_l) \right] = I_l - \mathbf{R}_l (a I'_l - B_l I_l), \quad (64)$$

or

$$U_l = \frac{I_l - \mathbf{R}_l (a I'_l - B_l I_l)}{-O_l + \mathbf{R}_l (a O'_l - B_l O_l)} = \frac{I_l}{O_l} \frac{1 - \mathbf{R}_l (a \frac{I'_l}{I_l} - B_l)}{1 - \mathbf{R}_l (a \frac{O'_l}{O_l} - B_l)}. \quad (65)$$

The logarithmic derivative L_l is defined as

$$L_l \equiv a \frac{O'_l}{O_l} = \left[R \frac{\partial \ln O_l}{\partial R} \right]_{R=a} \equiv S_l + i P_l. \quad (66)$$

For spinless particles, the complex conjugate relation $I_l^* = O_l$ can be used, so that

$$L_l^* \equiv a \frac{I'_l}{I_l} = \left[R \frac{\partial \ln I_l}{\partial R} \right]_{R=a} \equiv S_l - i P_l, \quad (67)$$

⁴For a more general derivation see Section VII.1 of [1]

and the ratio

$$\frac{I_l}{O_l} = \frac{O_l^*}{O_l} = \frac{|O_l| e^{-i\varphi_l}}{|O_l| e^{+i\varphi_l}} = e^{-2i\varphi_l}. \quad (68)$$

Therefore, Eq. (64) becomes

$$U_l = e^{-2i\varphi_l} \frac{1 - R_l(L_l^* - B_l)}{1 - R_l(L_l - B_l)}, \quad (69)$$

which is the usual form for the scattering matrix in terms of the R-matrix in this simple case.

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