Parameterization of Direct and Doorway Processes in R-Matrix Formalism

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Abstract. R-matrix formalism is extended beyond compound nuclear (CN) resonant reactions to include parameterization of direct as well as doorway processes. Direct processes in the R-matrix exterior are parameterized by a unitary matrix that introduces mixing among wave function coefficients of the incoming and outgoing wave function components at the R-matrix channel surface. Doorway processes are parameterized by separating the Hilbert space of the interior R-matrix region into its doorway and CN subspaces, from which doorway state eigenenergies, reduced width amplitudes, and the strengths of their coupling to CN levels appear as new R-matrix parameters. Parameterization of generalized as well as the conventional Reich–Moore approximation for eliminated capture channels in the presence of direct, doorway, and CN processes is presented along with a complex-valued scattering length with contributions from direct, doorway, and CN capture processes. Derivation of Brune’s alternative R-matrix parameters is extended to include doorway states. This work suggests how R-matrix formalism could be extended further by adopting the concepts from related reaction formalisms.

1 Introduction

A phenomenological R-matrix formalism reviewed by Lane and Thomas [1] has been used for evaluations of neutron cross sections [2, 3] in the resolved resonance region (RRR) compiled in the US Evaluated Nuclear Data File [4]. Inspired by formal expressions for the transition matrix accounting for direct, doorway, and compound nuclear (CN) processes in both the transition (T-)matrix formalism [5, 6] and the reactance (K-)matrix formalism [7], we introduce a corresponding parameterization of direct, doorway, and CN processes into a phenomenological R-matrix formalism. Because the R-matrix reaction channels include particle and radiative capture channels, these formal extensions enable R-matrix parameterization of three kinds of capture processes: direct, semidirect (via giant dipole resonances playing the role of doorways [10–12]), and CN capture processes, thus enabling quantum mechanical interference among them. These extensions also enable R-matrix doorway treatment of isobar analogue resonances (IARs) whose presence modulates neutron CN resonance widths [13] and capture cross sections [14].

Several expressions from the conventional phenomenological R-matrix formalism [1] are stated using bold font in matrix notation to facilitate the presentation of its formal extensions. A conventional expression for the scattering matrix in a phenomenological R-matrix formalism of CN processes presented by Lane and Thomas in [1] is

\[ U = \Omega W \Omega, \]

(1)

where \( \Omega \equiv e^{-i\phi(\rho)} \) is defined by a diagonal hard-sphere scattering phase shift matrix, \( \phi(\rho) \), where \( \rho \equiv ak \); \( a \) is a diagonal matrix of channel hard-sphere radii; \( k \) is a diagonal matrix of channel momentum wave numbers corresponding to a total energy, \( E \), in the center-of-mass frame; and the collision matrix, \( W \), is

\[ W = P^{\frac{1}{2}}[1 - R(L - B)]^{-1}[1 - R(L^* - B)] P^{-\frac{1}{2}}, \]

(2)

where \( L \) and \( L^* \) are diagonal matrices of logarithmic derivatives of (energy-dependent) outgoing (\( O \)) and incoming (\( I \)) channel wave functions, respectively; \( L \) is divided into its real and imaginary component, \( L \equiv S + iP \); \( L^* = S - iP \), that is, the shift function, \( S \), and the penetrability, \( P \), respectively; and \( B \) is a diagonal matrix of arbitrary real-valued boundary condition constants. Dimensions of all of the matrices above are \( (N_c \times N_c) \), where \( N_c = N_p + N_r \) is the total number of channels, and \( N_p \) and \( N_r \) are the number of particle and radiative capture channels, respectively. For later convenience, the R-matrix is

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1This is true for the various forms of the Reich–Moore approximation (RMA) [1, 8, 9] for eliminated capture channels described in Section 4.
expressed as
\[ R = \gamma \dagger Q \gamma, \quad (3) \]
\[ Q^{-1} = e - E1, \quad (4) \]
where \( e \) is a \((N_A \times N_A)\) diagonal matrix of CN level energies, \( \gamma \) is a \((N_A \times N_e)\) matrix of resonance reduced width amplitudes (RWAs), \( N_A \) is the number of CN levels, and the elements of \( e \) and \( \gamma \) are real parameters independent of energy, \( E \). The collision matrix, \( W \), in Eq. (2) can also be expressed as
\[ W = 1 + 2i P^2 \gamma^\dagger A \gamma P^3, \quad (5) \]
where \( A \) is a \((N_A \times N_A)\) level matrix expressed\(^2\) in terms of the R-matrix parameters as
\[ A^{-1} = Q^{-1} - \gamma (L - B) \gamma^\dagger. \quad (6) \]

Direct processes are introduced into R-matrix formalism in Section 2, doorway processes in Section 3, RMA of eliminated capture channels in the presence of direct and doorway process in Section 4, and the extension of Brune transform to doorway states in Section 5. Further extensions of R-matrix formalism enabled by these results are outlined in the conclusion.

2 Direct Processes in R-matrix Formalism

Direct reaction channel coupling in the R-matrix exterior suggested by Wigner [15] can be parameterized by a unitary matrix, \( M^{-1} = M^\dagger \equiv (M^\dagger)^\dagger \), that mixes the coefficients of the incoming, \( y \), and outgoing, \( x \), asymptotic channel wave function, \( \Psi = Iy + Ox \), at the R-matrix surface as
\[ y \leftarrow My \quad \text{and} \quad x \leftarrow M^\dagger x. \quad (7) \]
Substituting these into the R-matrix expression defining the scattering matrix, \( x = -My \), yields \( M^\dagger x = -UMy \); multiplying both sides by \( M^\dagger \) yields a unitary and symmetric\(^3\) scattering matrix modified for direct processes as
\[ U_M = M^\dagger UM, \quad (8) \]
where \( U \) in Eq. (8) retains the form given by Eqs. (1–4).

A slow energy variation of matrix elements of \( M \) over the energy scale on the order of optical potential single-particle resonance width—that is, 1 MeV—may be expected, suggesting that direct processes in the R-matrix interior could be parameterized by adapting the method of Section 3. An optimal form of parameterization could depend on the nature of a nuclear reaction. For example, unitary \( M \) can be parameterized by a Hermitian matrix \( \chi \) via \( M = \exp[-i\chi] \). Similarly, an orthonormal\(^4\) matrix may be parameterized by a skew-symmetric \( \gamma \) as \( M = \exp[\gamma] \).

Consistent R-matrix parameterization of direct processes introduced in this section and of doorway and CN processes in the next section enable a seamless quantum mechanical formalism for interference\(^5\) among the three classes of processes in all channels, as illustrated by an expression for the scattering length in Section 4.

3 Doorway States in R-matrix Formalism

A simple way to infer parameterization of doorway and CN processes in a phenomenological R-matrix is to cast the R-matrix resonance RWAs and energies in Eqs. (3) and (4), respectively, into an equivalent operator form as
\[ \gamma = \langle \lambda | c \rangle, \quad (9) \]
\[ e = \langle \lambda | H_0 | \lambda \rangle, \quad (10) \]
respectively, where \( | c \rangle \) and \( | \lambda \rangle \) are the eigenvectors of (channel radius sphere) surface and interior states, respectively, and \( H_0 \) is a Hamiltonian of the interior [5].

The interior Hilbert space, \( | \lambda \rangle \), is to be delineated into a subspace of compound nuclear states, \( | q \rangle \), and a subspace of doorway states, \( | d \rangle \), orthogonal to it, \( \langle d | \langle q | = 0 \). This can be achieved by making a formal substitution\(^6\),
\[ \langle \lambda | \leftarrow \langle d |, \quad \langle q | \leftarrow \langle q |, \quad (11) \]
in Eqs. (9) and (10) to obtain the following generalizations of \( \gamma \) and \( e \) for use in Eq. (3) and Eq. (4), respectively\(^7\):
\[ \gamma \leftarrow \gamma_d\gamma_q, \quad (12) \]
\[ \gamma_d \equiv \langle d | c \rangle \quad \text{and} \quad \gamma_q \equiv \langle q | c \rangle \quad (13) \]
are the RWA matrices of doorway and CN states, respectively, and
\[ e \leftarrow \begin{pmatrix} e_d & v \\ v^\dagger & e_q \end{pmatrix}, \quad 1 \leftarrow \begin{pmatrix} 1_d & 0 \\ 0 & 1_q \end{pmatrix}. \quad (14) \]
where\(^8\)
\[ v \equiv \langle d | H | q \rangle, \quad e_d \equiv \langle d | H | d \rangle, \quad e_q \equiv \langle q | H | q \rangle. \quad (15) \]
are a doorway–CN level coupling strength matrix, followed by diagonal matrices of doorway and CN level energies, respectively. Although \( e_d \) and \( e_q \) are diagonal, a \((2 \times 2)\) block matrix \( e \) is not because of the non-vanishing off-diagonal blocks \( v \) and \( v^\dagger \). The \( R \) - and \( A \)-matrix in Eqs. (3) and (6), respectively, attain a \((2 \times 2)\) block matrix structure due to Eqs. (12, 14). All matrix elements of \( e \) (including those of its constituent \( v \)) and \( \gamma \) remain real-valued and independent of energy, \( E \).

A projection of the R-matrix interior Hilbert space by Eq. (11) was inspired by Feshbach’s projector operator formalism [5], and it turns out to be particularly simple because it is applied to a denominator\(^9\) of the \( Q \)-matrix, instead of the \( R \)-matrix, that is, the Green’s function [6, 7].

\(^2\)The fact that the expression in Eq. (6) holds for any real symmetric matrix \( e \) is used in the generalized RMA in Section 4 and for alternative R-matrix parameterization in Section 5.

\(^3\)See Section VI.2.a,b of [1] for more information.

\(^4\)It is an R-matrix analogue for the orthonormal matrix (computed via distorted wave approx.) in Eq. (III.2.26) of [5] in \( T \)-matrix formalism.

\(^5\)This interference may be constructive or destructive.

\(^6\)The choice of the letters \( "d" \) and \( "q" \) to label doorway and compound level subspaces is borrowed from [5–7].

\(^7\)Matrix subscripts \( (d, q, ...) \) serve as labels rather than indices.

\(^8\)A two-nucleon component of a nuclear Hamiltonian can induce a chain of linked subspaces of increasing number of particle-holes [16].

\(^9\)More specifically, the matrix \( e \) inside the denominator.
4 Approximations for Capture Channels

Approximations of R-matrix total capture cross section in the presence of direct, doorway, and CN processes must be performed simultaneously for all three classes of processes. Formal elimination of capture channels starts with doorway and CN processes, followed by a corresponding elimination of direct processes.

Application of generalized RMA (GRMA) [9] to the last term of a $(2 \times 2)$ block-level matrix in Eq. (6) reduces the total number of channels, $N_c = N_p + N_f$—where $N_p$ and $N_f$ are the number of particle and radiative capture channels, respectively—to $N_{GRMA} = N_p + N_d$, where $N_d$ is a total number of levels, including doorway and CN levels, namely, $N_d = N_q + N_d$. Since the expressions derived in [9] hold for any symmetric matrix $e$, including the one defined by Eq. (14), a matrix of GRMA RWAs for the $N_d$ surrogate capture channels is

\[
g_q = \gamma_q P^{1/2} P^{1/2} \gamma_q,
\]

where $g_q$ is a $N_d \times N_d$ symmetric matrix of GRMA surrogate RWAs [9], and $\gamma_q$ is the original, presumably complete, $(N_q \times N_q)$ matrix of RWAs.

This reduction in number of capture channels entails a corresponding reduction for direct processes, governed by

\[
g_p\gamma_p = \gamma_p P^{1/2} \gamma_p P^{1/2} P^{1/2} \gamma_p,
\]

where $M_v$ is a $(N_p \times N_p)$ off-diagonal block matrix in a $(N_q \times N_q)$ direct reaction matrix $M$, to be replaced by $m_v$, a $(N_f \times N_f)$ matrix. This reduced set of surrogate capture channel parameters, $(g_q, m_v)$, can reproduce a total capture cross section computed using a complete parameter set, $(\gamma_q, M_v)$. When a complete set of capture RWAs is not known, one may simply perform evaluation using a surrogate set, $(g_q, m_v)$. The GRMA parameters remain real-valued, and the corresponding scattering matrix therefore remains unitary. The Brune transform developed in Section 5 can be applied directly to the GRMA parameterization [9].

Conventional RMA sets to zero all off-diagonal elements (presumed to be small) of $g_q$ to yield

\[
e(RMA) = e - i \cdot \text{diag}(g_q^2).
\]

A corresponding RMA for eliminated DC can be stated via a skew-symmetric matrix $\chi$ corresponding to the orthonormal matrix $M = \exp(\chi)$. For example, for a single $s$-wave elastic channel in the limit $k_0 \rightarrow 0$, the loss of incoming flux due to DC can be parameterized by $\phi_0 > 0$ as

\[
\chi(RMA) = -\phi_0 \phi_0 \gamma_q = -\phi_0 \gamma_q - i \gamma_q,
\]

to yield an expression for a free scattering length as

\[
a(RMA) \equiv \lim_{k_0 \rightarrow 0} \frac{1}{2ik_0} (1 - U_{MB}) \approx a_0 [1 - \gamma_q e^{i\phi(RMA)} \gamma_q - i\gamma_q^2],
\]

where $-i\phi(RMA)$ is a DC contribution to the imaginary part of the scattering length, which parameterizes capture cross section in the thermal neutron region as $-4\pi|a_{GRMA}|/k_0$. Its absolute value parameterizes a corresponding scattering cross section in the center of mass frame as $4\pi|a_{GRMA}|^2$. The expression for a free scattering length in Eq. (20), being related to the bound scattering lengths used in thermal neutron scattering (TNS) evaluations [17], could be used to correlate presently uncorrelated TNS and RRR evaluations.

5 Alternative R-matrix for Doorways

The Brune transform of conventional (real-valued) $R$-matrix resonance parameters to alternative $R$-matrix parameters [18] is extended to include the doorway states introduced into $R$-matrix formalism in Section 3. Brune transform may be performed on doorway and CN subspaces independently to yield alternative parameter sets for each subspace: $\tilde{\chi}(d), \tilde{\gamma}(d)$, and $\tilde{\gamma}(q)$, respectively. To complete the Brune transform in the presence of doorway states, it remains to transform the doorway–CN level coupling matrix, $\gamma$, in Eq. (15), which is the off-diagonal block matrix of the $(2 \times 2)$ block matrix $\gamma$ given by Eq. (14). This is achieved by generalizing the matrices defined in the Brune [18] derivation, namely, $E, M, N, A, \rho$, and $\bar{Q}$, which become $(2 \times 2)$ block matrices due to the introduction of the doorway subspace. The matrix, $E$, introduced by Brune becomes implicitly generalized into a $(2 \times 2)$ block matrix, namely,

\[
E = e - \gamma (S - B) \gamma^T,
\]

by virtue of $\gamma$ and $e$ having already been redefined as $(2 \times 1)$ and $(2 \times 2)$ block matrices in Eqs. (12) and (14), respectively. A generalization of Brune’s eigenvector matrix for a projected Hilbert space is a $2 \times 2$ block-diagonal matrix

\[
a = a_d \otimes a_q = \begin{pmatrix} a_d & 0 \\ 0 & a_q \end{pmatrix},
\]

where $a_d$ is the eigenvector matrix introduced by Brune [18] of the CN (doorway) subspace. The length of each eigenvector in $a$ is $(N_q + N_d)$. The product space of eigenvectors in Eq. (22) may be used to succinctly define the alternative RWAs as

\[
\tilde{\gamma} = a \gamma = \begin{pmatrix} \tilde{\gamma}_d \\ \tilde{\gamma}_q \end{pmatrix} = \begin{pmatrix} a_d \gamma_d \\ a_q \gamma_q \end{pmatrix}.
\]

The eigenvector overlap matrix, $M$, is extended via Eq. (22) as

\[
M = a^\dagger a = \begin{pmatrix} M_d & 0 \\ 0 & M_q \end{pmatrix},
\]

and

\[
N = a^\dagger e a = \begin{pmatrix} N_d & N_{dq} \\ N_{qd}^\dagger & N_q \end{pmatrix},
\]

where $M_{(dq)}$ and $N_{(dq)}$ retain the form derived in [18], and

\[
N_q = \tilde{\gamma}_q (S - B) \tilde{\gamma}_q^T.
\]
where
\[ \vec{b} = a_q a^\dagger_i. \]
and the \((i, j)\) matrix element of \(\vec{S}\) is
\[ [\vec{S}]_{ij} = \frac{S[(\vec{r}_d)_i] + S[(\vec{r}_q)_j]}{2}. \]
The Brune transform of the level matrix in Eq. (6) yields
\[ \vec{A}^{-1} = a^\dagger A^{-1} a = N - EM - \gamma(L - B)\gamma^\dagger \]
\[ = \vec{Q}^{-1} - i\gamma\tilde{P}\gamma^\dagger \]
which can be solved for \(\vec{Q}^{-1}\) using Eqs. (30, 31, 24-28) to yield
\[ \vec{Q}^{-1} = \begin{pmatrix} [\vec{Q}^{-1}]_d & [\vec{Q}^{-1}]_o \\ [\vec{Q}^{-1}]_o & [\vec{Q}^{-1}]_d \end{pmatrix}, \]
where \([\vec{Q}^{-1}]_d\) and \([\vec{Q}^{-1}]_o\) correspond to \(\vec{Q}^{-1}(E)\) of [18] for parameter sets \((\vec{r}_d, \gamma_d)\) and \((\vec{r}_q, \gamma_q)\), respectively, and where
\[ [\vec{Q}^{-1}]_o = \vec{b} - \gamma_1[S(E) - \tilde{S}\gamma]^\dagger. \]

Brune’s alternative R-matrix, namely, \(\tilde{R} = \gamma^\dagger \vec{Q}\gamma\), can be used to express the collision matrix \(W\) in Eq. (2) as
\[ W = [1 - iP^2 \tilde{R}P^2]^{-1}[1 + iP^2 \tilde{R}P^2]. \]

6 Summary and Outlook

Direct and doorway processes have been seamlessly parameterized in a phenomenological R-matrix formalism, including a corresponding RMA and the Brune transform. It is hoped that incorporating these processes into R-matrix nuclear data evaluation codes such as SAMMY [2, 3] will yield improved evaluations for nuclear applications.

Introduction of doorway processes into the R-matrix suggests that further subdivisions of the interior R-matrix Hilbert space could yield an R-matrix analog of the Feshbach–Kerman–Koonin theory of multistep compound nuclear reactions [16, 20]; each subspace induced by a particle-hole pair (2p1h, 3p2h, ...) would entail a row and column block into a block matrix \(\vec{Q}\) in Eq. (32) (using expressions in [19]) is analogous to the \((2 \times 2)\) block components of a \(K\)-matrix derived using projection operator formalism in [6]. A notion that this correspondence could be established lead to a transparent R-matrix parameterization of doorway processes in Section 3.

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