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 Rmatrix formalism. Because the *R*-matrix reaction channels include particle and radiative capture channels, these formal extensions enable R-matrix parameterization of three kinds of capture¹ 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 of [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

$$\boldsymbol{U} = \boldsymbol{\Omega} \boldsymbol{W} \boldsymbol{\Omega}, \tag{1}$$

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

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

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 $N_c = N_p + N_\gamma$ is the total number of channels, and N_p and N_γ 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

$$\boldsymbol{R} = \boldsymbol{\gamma}^{\mathsf{T}} \boldsymbol{Q} \, \boldsymbol{\gamma}, \qquad (3)$$

$$\boldsymbol{Q}^{-1} = \boldsymbol{e} - E \boldsymbol{1}, \qquad (4)$$

where e is a $(N_{\lambda} \times N_{\lambda})$ diagonal matrix of CN level energies, γ is a $(N_{\lambda} \times N_c)$ matrix of resonance reduced width amplitudes (RWAs), N_{λ} is the number of CN levels, and the elements of e and γ are real parameters independent of energy, E. The collision matrix, W, in Eq. (2) can also be expressed as

$$\boldsymbol{W} = \boldsymbol{1} + 2\,\boldsymbol{i}\,\boldsymbol{P}^{\frac{1}{2}}\,\boldsymbol{\gamma}^{\mathsf{T}}\boldsymbol{A}\,\boldsymbol{\gamma}\,\boldsymbol{P}^{\frac{1}{2}},\tag{5}$$

where *A* is a $(N_{\lambda} \times N_{\lambda})$ *level* matrix expressed² in terms of the *R*-matrix parameters as

$$\boldsymbol{A}^{-1} = \boldsymbol{Q}^{-1} - \boldsymbol{\gamma} \left(\boldsymbol{L} - \boldsymbol{B} \right) \boldsymbol{\gamma}^{\mathsf{T}}.$$
 (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 *uni-tary* matrix, $\mathcal{M}^{-1} = \mathcal{M}^{\dagger} \equiv (\mathcal{M}^*)^{\intercal}$, that mixes the coefficients of the incoming, y, and outgoing, x, asymptotic channel wave function, $\Psi = Iy + Ox$, at the *R*-matrix *surface* as

$$\boldsymbol{y} \leftarrow \mathcal{M} \, \boldsymbol{y} \quad \text{and} \quad \boldsymbol{x} \leftarrow \mathcal{M}^* \, \boldsymbol{x}.$$
 (7)

Substituting these into the *R*-matrix expression defining the scattering matrix, x = -Uy, yields $\mathcal{M}^* x = -U\mathcal{M} y$; multiplying both sides by \mathcal{M}^{T} yields a unitary and symmetric³ scattering matrix modified for direct processes as

$$U_{\mathcal{M}} = \mathcal{M}^{\mathsf{T}} U \mathcal{M}, \tag{8}$$

where U in Eq. (8) retains the form given by Eqs. (1–4).

A slow energy variation of matrix elements of \mathcal{M} over the energy scale on the order of optical potential singleparticle 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 \mathcal{M} can be parameterized by a Hermitian matrix χ via $\mathcal{M} = \exp[-i\chi]$. Similarly, an orthonormal⁴ matrix may be parameterized by a skew-symmetric χ as $\mathcal{M} = \exp[\chi]$.

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 interference⁵ 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

$$\boldsymbol{\gamma} = \langle \boldsymbol{\lambda} | \boldsymbol{c} \rangle, \tag{9}$$

$$\boldsymbol{e} = \langle \boldsymbol{\lambda} | \boldsymbol{H}_0 | \boldsymbol{\lambda} \rangle, \qquad (10)$$

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, $\langle d|\otimes |q\rangle = 0$. This can be achieved by making a formal substitution⁶,

$$\langle \lambda | \leftarrow \begin{pmatrix} \langle d | \\ \langle q | \end{pmatrix},$$
 (11)

in Eqs. (9) and (10) to obtain the following generalizations of γ and e for use in Eq. (3) and Eq. (4), respectively⁷:

$$\gamma \leftarrow \begin{pmatrix} \gamma_d \\ \gamma_q \end{pmatrix}$$
, where (12)

$$\gamma_d \equiv \langle d | c \rangle$$
 and $\gamma_q \equiv \langle q | c \rangle$ (13)

are the RWA matrices of doorway and CN states, respectively, and

$$e \leftarrow \begin{pmatrix} e_d & v \\ v^{\mathsf{T}} & e_q \end{pmatrix}, \quad \mathbf{1} \leftarrow \begin{pmatrix} \mathbf{1}_d & \mathbf{0} \\ \mathbf{0}^{\mathsf{T}} & \mathbf{1}_q \end{pmatrix},$$
 (14)

where⁸

$$\boldsymbol{v} \equiv \langle d | \boldsymbol{H} | q \rangle, \quad \boldsymbol{e}_{d} \equiv \langle d | \boldsymbol{H} | d \rangle, \quad \boldsymbol{e}_{q} \equiv \langle q | \boldsymbol{H} | q \rangle, \quad (15)$$

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 (2×2) block matrix e is not because of the non-vanishing off-diagonal blocks v and v^{\intercal} . The R- and A-matrix in Eqs. (3) and (6), respectively, attain a 2×2 block matrix structure due to Eqs. (12, 14). All matrix elements of e (including those of its constituent v) and γ 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].

²The 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.

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

⁴It 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.

⁵This interference may be constructive or destructive.

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

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

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

⁹More 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 × 2) block-level matrix in Eq. (6) reduces the total number of channels, $N_c = N_p + N_\gamma$ —where N_p and N_γ are the number of particle and radiative capture channels, respectively—to $N_{\text{GRMA}} = N_p + N_\lambda$, where N_λ is a total number of levels, including doorway and CN levels, namely, $N_\lambda = N_q + N_d$. 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_λ surrogate capture channels is

$$\boldsymbol{g}_{\gamma}^{2} = \boldsymbol{\gamma}_{\gamma}^{\mathsf{T}} \boldsymbol{P}_{\gamma}^{1/2} \boldsymbol{P}_{\gamma}^{1/2} \boldsymbol{\gamma}_{\gamma}, \qquad (16)$$

where g_{γ} is a $N_{\lambda} \times N_{\lambda}$ symmetric matrix¹⁰ of GRMA surrogate RWAs [9], and γ_{γ} is the original, presumably complete, $(N_{\gamma} \times N_{\lambda})$ matrix of RWAs.

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

$$\boldsymbol{g}_{\gamma}\boldsymbol{m}_{\gamma} = \boldsymbol{\gamma}_{\gamma}^{\mathsf{T}} \boldsymbol{P}_{\gamma}^{1/2} \mathcal{M}_{\gamma}, \qquad (17)$$

where \mathcal{M}_{γ} is a $(N_{\gamma} \times N_{p})$ off-diagonal block matrix in a $(N_{c} \times N_{c})$ direct reaction matrix \mathcal{M} , to be replaced by m_{γ} , a $(N_{\lambda} \times N_{p})$ matrix. This reduced set of surrogate capture channel parameters, (g_{γ}, m_{γ}) , can reproduce a total capture cross section computed using a complete parameter set, $(\gamma_{\gamma}, \mathcal{M}_{\gamma})$. When a complete set of capture RWAs is not known, one may simply perform evaluation using a surrogate set, (g_{γ}, m_{γ}) . 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 small¹¹) of g_{γ} to yield

$$\boldsymbol{e}_{(\text{RMA})} = \boldsymbol{e} - i \cdot \text{diag}(\boldsymbol{g}_{\gamma}^2). \tag{18}$$

A corresponding RMA for eliminated DC can be stated via a skew-symmetric matrix χ corresponding to the orthonormal matrix $\mathcal{M} = \exp(\chi)$. For example, for a single *s*-wave elastic channel¹² in the limit $k_0 \rightarrow 0$, the loss of incoming flux due to DC can be parameterized¹³ by $\varepsilon_0 > 0$ as

$$\chi_{0(\text{RMA})} = -\varepsilon_0 \phi_0(\rho_0) = -\varepsilon_0 a_0 k_0, \tag{19}$$

to yield an expression for a free scattering length¹⁴ as

$$a_{(\text{RMA})} \equiv \lim_{k_0 \to 0} \frac{1}{2ik_0} (1 - \boldsymbol{U}_{\mathcal{M}0}) \approx a_0 [1 - \boldsymbol{\gamma}_0^{\mathsf{T}} \boldsymbol{e}_{(\text{RMA})}^{-1} \boldsymbol{\gamma}_0 - i\varepsilon_0],$$
(20)

where $-ia_0\varepsilon_0$ is a DC contribution to the imaginary part of the scattering length¹⁵, which parameterizes capture cross section in the thermal neutron region as $-4\pi\Im[a_{(RMA)}]/k_0$. Its absolute value parameterizes a corresponding scattering cross section in the center of mass frame as $4\pi|a_{(RMA)}|^2$. 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) Rmatrix 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: $(\tilde{\boldsymbol{e}}_d, \tilde{\boldsymbol{\gamma}}_d)$ and $(\tilde{\boldsymbol{e}}_q, \tilde{\boldsymbol{\gamma}}_q)$, respectively. To complete the Brune transform in the presence of doorway states, it remains to transform the doorway-CN level coupling matrix, \boldsymbol{v} , in Eq. (15), which is the off-diagonal block matrix of the (2×2) block matrix *e* given by Eq. (14). This is achieved by generalizing the matrices defined in the Brune [18] derivation, namely, \mathcal{E} , M, N, \tilde{A} , and \tilde{Q} , which become (2×2) block matrices due to the introduction of the doorway subspace. The matrix, &, introduced by Brune becomes implicitly generalized into a (2×2) block matrix, namely,

$$\mathcal{E} = \boldsymbol{e} - \boldsymbol{\gamma} \left(\boldsymbol{S} - \boldsymbol{B} \right) \boldsymbol{\gamma}^{\mathsf{T}},\tag{21}$$

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

$$\boldsymbol{a} = \boldsymbol{a}_d \otimes \boldsymbol{a}_q = \begin{pmatrix} \boldsymbol{a}_d & \boldsymbol{0} \\ \boldsymbol{0}^{\mathsf{T}} & \boldsymbol{a}_q \end{pmatrix}, \tag{22}$$

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

$$\tilde{\boldsymbol{\gamma}} = \boldsymbol{a}\boldsymbol{\gamma} = \begin{pmatrix} \tilde{\boldsymbol{\gamma}}_d \\ \tilde{\boldsymbol{\gamma}}_q \end{pmatrix} = \begin{pmatrix} \boldsymbol{a}_d \boldsymbol{\gamma}_d \\ \boldsymbol{a}_q \boldsymbol{\gamma}_q \end{pmatrix}.$$
(23)

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

$$\boldsymbol{M} = \boldsymbol{a}^{\mathsf{T}} \boldsymbol{a} = \begin{pmatrix} \boldsymbol{M}_d & \boldsymbol{0} \\ \boldsymbol{0}^{\mathsf{T}} & \boldsymbol{M}_q \end{pmatrix},$$
(24)

and

$$\mathbf{N} = \mathbf{a}^{\mathsf{T}} \mathbf{e} \mathbf{a} = \begin{pmatrix} N_d & N_v \\ N_v^{\mathsf{T}} & N_q \end{pmatrix}, \tag{25}$$

where $M_{\{d,q\}}$ and $N_{\{d,q\}}$ retain the form derived in [18], and

$$N_{v} \equiv \tilde{\boldsymbol{v}} + \tilde{\boldsymbol{\gamma}}_{d} (\bar{\boldsymbol{S}} - \boldsymbol{B}) \tilde{\boldsymbol{\gamma}}_{q}^{\mathsf{T}}, \qquad (26)$$

¹⁰Its (2×2) block structure in Eq. (12) remains.

¹¹Asymptotically true when assuming randomly distributed signs of capture RWAs, γ_{γ} , and direct capture (DC) amplitudes, \mathcal{M}_{γ} , and $N_{\gamma} \gg 1$. ¹²Labeled as subscript 0, *e.g.*, a_0 is its *R*-matrix channel radius.

¹³A total capture cross section is then proportional to a deviation of the scattering matrix from unitarity [2].

¹⁴The off-diagonal elements of g_{γ}^2 may be kept in Eq. (18), as in [1].

¹⁵Doorway states and CN levels contribute via $e_{(RMA)}$.

where

$$\tilde{\boldsymbol{v}} = \boldsymbol{a}_d \boldsymbol{v} \boldsymbol{a}_q^{\mathsf{T}},\tag{27}$$

and the (i, j) matrix element of \bar{S} is

$$[\bar{\boldsymbol{S}}]_{ij} \equiv \frac{\boldsymbol{S}([\tilde{\boldsymbol{e}}_d]_{ii}) + \boldsymbol{S}([\tilde{\boldsymbol{e}}_q]_{jj})}{2}.$$
 (28)

The Brune transform of the level matrix in Eq. (6) yields

$$\tilde{A}^{-1} = a^{\mathsf{T}} A^{-1} a \tag{29}$$

$$= N - EM - \tilde{\gamma}(L - B)\tilde{\gamma}^{\mathsf{T}}$$
(30)

$$= \tilde{\boldsymbol{Q}}^{-1} - i\tilde{\boldsymbol{\gamma}}\boldsymbol{P}\tilde{\boldsymbol{\gamma}}^{\mathsf{T}}$$
(31)

which can be solved for \tilde{Q}^{-1} using Eqs. (30, 31, 24-28) to yield

$$\tilde{\boldsymbol{\mathcal{Q}}}^{-1} = \begin{pmatrix} [\tilde{\boldsymbol{\mathcal{Q}}}^{-1}]_d & [\tilde{\boldsymbol{\mathcal{Q}}}^{-1}]_v \\ [\tilde{\boldsymbol{\mathcal{Q}}}^{-1}]_v^{\mathsf{T}} & [\tilde{\boldsymbol{\mathcal{Q}}}^{-1}]_q \end{pmatrix}, \tag{32}$$

where $[\tilde{\boldsymbol{Q}}^{-1}]_d$ and $[\tilde{\boldsymbol{Q}}^{-1}]_q$ correspond to $\tilde{\boldsymbol{Q}}^{-1}(E)$ of [18] for parameter sets $(\tilde{\boldsymbol{e}}_d, \tilde{\boldsymbol{\gamma}}_d)$ and $(\tilde{\boldsymbol{e}}_q, \tilde{\boldsymbol{\gamma}}_q)$, respectively, and where

$$[\tilde{\boldsymbol{Q}}^{-1}]_v = \tilde{\boldsymbol{v}} - \tilde{\boldsymbol{\gamma}}_d [\boldsymbol{S}(E) - \bar{\boldsymbol{S}}] \tilde{\boldsymbol{\gamma}}_q^{\mathsf{T}}.$$
(33)

Brune's alternative *R*-matrix, namely, $\tilde{R} = \tilde{\gamma}^{\mathsf{T}} \tilde{Q} \tilde{\gamma}$, can be used to express the collision matrix *W* in Eq. (2) as

$$W = [1 - iP^{\frac{1}{2}}\tilde{R}P^{\frac{1}{2}}]^{-1}[1 + iP^{\frac{1}{2}}\tilde{R}P^{\frac{1}{2}}], \qquad (34)$$

suggesting that $P^{\frac{1}{2}}\tilde{R}P^{\frac{1}{2}}$ corresponds to a *K*-matrix; in fact, a formal structure of its (2×2) block components (obtained by formally inverting a (2×2) block matrix \tilde{Q}^{-1} in Eq. (32) (using expressions in [19]) is analogous to the (2×2) block components of a *K*-matrix derived using projection operator formalism in [6]. A notion that this correspondence could be established led to a transparent *R*-matrix parameterization of doorway processes in Section 3.

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 *e* in Eq. (14). A corresponding scattering matrix could be computed without any approximations because the formal complexity has been contained inside the computation of a matrix inverse of a block-matrix (*e*–*E*1) that can be performed by computers.

Addition of direct and doorway processes into a CN formalism enables a relaxation of the assumptions inherent to applications of random matrix theory in nuclear physics [21, 22], and it may be useful for advancing statistical methods in the *R*-matrix formalism for the unresolved resonance region, where fluctuations suggestive of intermediate structure induced by doorway states are seen [5, 13].

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