Generalized Reich-Moore $R$-matrix approximation

Goran Arbanas 1,2, Vladimir Sobes 1, Andrew Holcomb 1, Pablo Ducru 2, Marco Pigni 1, and Dorothea Wiarda 1

1 Nuclear Data and Criticality Safety Group, Reactor and Nuclear Systems Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6171, USA
2 Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Abstract. A conventional Reich-Moore approximation (RMA) of $R$-matrix is generalized into a manifestly unitary form by introducing a set of resonant capture channels treated explicitly in a generalized, reduced $R$-matrix. A dramatic reduction of channel space witnessed in conventional RMA, from $N_c \times N_c$ full $R$-matrix to $N_p \times N_p$ reduced $R$-matrix, where $N_c = N_p + N_r$, $N_p$ and $N_r$ denoting the number of particle and $\gamma$-ray channels, respectively, is due to $N_p \ll N_r$. A corresponding reduction of channel space in generalized RMA (GRMA) is from $N_c \times N_c$ full $R$-matrix to $N_{GRMA} \times N_{GRMA}$, where $N_{GRMA} = N_p + N_{GRMA}$, and where $N_{GRMA}$ is the number of capture channels defined in GRMA. We show that $N_{GRMA} = N_p$, where $N_p$ is the number of $R$-matrix levels. This reduction in channel space, although not as dramatic as in the conventional RMA, could be significant for medium and heavy nuclides where $N_{GRMA} \ll N_r$. The resonant capture channels defined by GRMA accommodate level-level interference (via capture channels) neglected in conventional RMA. The expression for total capture cross section in GRMA is formally equal to that of the full $N_c \times N_c$ $R$-matrix. This suggests that GRMA could yield improved nuclear data evaluations in the resolved resonance range at a cost of introducing $N_{GRMA}(N_{GRMA} - 1)/2$ resonant capture width parameters relative to conventional RMA. Manifest unitarity of GRMA justifies a method advocated by Fröhner and implemented in the SAMMY nuclear data evaluation code for enforcing unitarity of conventional RMA. Capture widths of GRMA are exactly convertible into alternative $R$-matrix parameters via Brune transform. Application of idealized statistical methods to GRMA shows that variance among conventional RMA capture widths in extant RMA evaluations could be used to estimate variance among off-diagonal elements neglected by conventional RMA. Significant departure of capture widths from an idealized distribution may indicate the presence of underlying doorway states.

1. Introduction

A phenomenological $R$-matrix formalism [1–4] has been used extensively for fitting $R$-matrix resonance parameters to resolved and unresolved resonance energy ranges of neutron-induced cross section data [5,6]. This formalism has recently been used for charged-particle cross section data [7]. For medium and heavy nuclides, Reich-Moore approximation (RMA) provides a statistically motivated approximation to total capture cross section by neglecting level-level interference via capture channels [8], thus conveniently replacing a multitude of capture widths of the full $R$-matrix by a single total capture width per resonance. In this work, RMA is formally generalized by retaining level-level interference via capture channels that are neglected in the conventional RMA. In this generalization the reduced number of capture channels, $N_{GRMA}^c$, turns out to be equal to the number of levels $N_p$. Diagonal elements of GRMA capture width matrix correspond to capture widths in the conventional RMA. Potential benefits, implications, and drawbacks of generalized GRMA are discussed.

Section 2 shows that expressions for the total capture and non-capture cross sections of the GRMA are formally equal to those of the full $R$-matrix. Section 3 shows that GRMA formalism, and consequently the conventional RMA formalism, is formally unitary and supports the prescription by F. Fröhner [3] for enforcing unitarity of the conventional RMA implemented in the nuclear data evaluation code SAMMY [6]. Statistical properties of matrix elements of GRMA’s reduced capture-width matrix are discussed in Sect. 4. Section 5 provides a formula for converting generalized Reich-Moore resonance parameters into alternative $R$-matrix parameters defined via Brune transform [9]. Notation is summarized in the Appendix.

2. Formalism

Cross sections may be expressed in a matrix form, $\sigma \equiv \{\sigma_{\alpha c}, c\}$, where the incoming channel $c = \{\alpha, J, l, s\}$ and the outgoing channel $c'$ are defined by a channel’s particle-pair ($\alpha$), threshold energy ($E^*$), orbital angular momentum...
(l), channel spin (s), and total angular momentum (J) quantum numbers, as
\[
\sigma = \frac{\pi}{k_0^2} g_{\lambda \mu \nu} |w_c|^{-2} U |e^{-j \delta_{j'}} - 1|^{-2} \delta_{j'},
\]
where \(k_0\) is the projectile’s momentum wave number in the center of mass frame, \(g_{\lambda \mu \nu} = (2j + 1) ![2j + 1](2j + 1)\) is the spin-statistical factor (i and J are the intrinsic spin of the projectile and the target, respectively), and \(w_c\) is a Coulomb scattering phase-shift in channel \(c\). The scattering matrix \(U\)
\[
U = \Omega(1 + 2i P^{1/2} \gamma^T A \gamma P^{1/2}) \Omega
\]
is conveniently expressed via level matrix \(A\)
\[
A^{-1} = e - E_1 + \gamma(L - B) \gamma^T,
\]
where \(e\) is a \((N_x \times N_x)\) diagonal matrix containing \(R\)-matrix resonance energies along its diagonal, and matrix elements of diagonal matrix \(\Omega\) are \(\Omega_{g\nu} = g_{\lambda \mu \nu} \exp[i(w_c - \phi_c)],\) where \(\phi_c\) is the hard-sphere phase-shift in channel \(c\).

The complete partial width amplitude \((N_x \times N_x)\) matrix \(\gamma\) shown above, where \(N_x = N_p + N_g\), is separated into its particle channel \((N_x \times N_p)\) sub-matrix \(\gamma_p\) and its \(\gamma\)-ray channel \((N_x \times N_g)\) sub-matrix \(\gamma_g\).
\[
\gamma \equiv (\gamma_p, \gamma_g).
\]

Similarly, diagonal matrix \(L - B\) is separated analogously
\[
L - B = \begin{pmatrix} L_p - B_p & 0 \\ 0 & L_g - B_g \end{pmatrix}
\]
so that a level matrix \(A\) could be expressed as
\[
A^{-1} = e - E_1 + \gamma_p(L_p - B_p) \gamma_p^T + \gamma_g(L_g - B_g) \gamma_g^T,
\]
where \(L_p\) are logarithmic derivatives of \(\gamma\)-ray outgoing wave functions separated into its real and imaginary parts, namely, shift function \(S_p \equiv \Re(L_p)\) and penetrability \(P_p \equiv \Im(L_p),\) and where \(B_p\) are the boundary conditions. Approximating the shift factor of \(\gamma\)-ray channels by 0 and setting their boundary conditions to 0 yields
\[
L_p - B_p \equiv S_p + i P_p - B_p \approx i P_p,
\]
while particle-related \(S_p\) and \(P_p\) are computed via Coulomb functions [4]. Consequently, the level matrix \(A\) could be written as
\[
A^{-1} \approx e - E_1 + i \gamma_p P_p^{1/2} \gamma_p^T + \gamma_g(L_p - B_p) \gamma_g^T
\]
where \(\gamma\)-ray penetrability \(P_p\) has been written as a product of penetrability amplitude \(P_p^{1/2} = (a_k k_j)^{-1/2}\), where \(L_j\) is a \(\gamma\)-ray multipolarity, \(a_k\) is its channel radius, and \(k\) is its momentum wavenumber, so that \(E = \hbar k c\) is its energy [10,11]. Any one of \(N_e\) \(\gamma\)-ray channels is specified by the energy \(E_j\) and quantum numbers \((J_j, M_j, \pi_j)\) of the level into which neutron is captured by emission of a primary \(\gamma\)-ray, and, by the quantum numbers (multipolarity, its projection, and the parity) of that primary \(\gamma\)-ray, \((L_j, M_j, \pi_j)\). For convenience, generalized Reich-Moore capture width \((N_x \times N_x)\) matrix is defined as
\[
\Gamma^{(6p)}(\gamma) / 2 \equiv \gamma_p P_p^{1/2} \gamma_p^T + \gamma_g B_g \gamma_g^T
\]
in terms of Eq. (8) becomes
\[
A^{-1} = e - E_1 + i \Gamma^{(6p)}(\gamma) / 2 + \gamma_g B_g \gamma_g^T.
\]
Conventional RMA assumes that the destructive interference\(^1\) of a multitude of \(N_e\) capture channels would render the off-diagonal elements of \(\Gamma^{(6p)}(\gamma)\) much smaller in magnitude than its (always positive) diagonal elements. Consequently, in conventional RMA \(\Gamma^{(6p)}(\gamma)\) is approximated by a purely diagonal matrix whose diagonal elements are the conventional RMA capture widths. In contrast to this, GRMA explicitly retains the off-diagonal elements of \(\Gamma^{(6p)}(\gamma)\) defined above. These non-vanishing off-diagonal elements could be computed, if the details of all \(N_e\) \(\gamma\)-ray channels were known. However, in the context of phenomenological R-matrix formalism where the aim is to fit cross section data rather than to predict it, these off-diagonal elements are viewed simply as theoretically motivated parameters that are to be determined solely by fitting to cross section data. That is, fitting those parameter does not require knowledge of underlying \(N_e\) capture channels.

It is advantageous to observe that capture width matrix \(\Gamma^{(6p)}(\gamma)\) is positive semidefinite thanks to its form \(M^T M\). This property guarantees that its principal root could be computed to yield a reduced and symmetric \((N_x \times N_x)\) matrix of capture width amplitudes
\[
\gamma_p' \equiv \Gamma^{(6p)}(\gamma) / 2^{1/2}.
\]
Since dimension of \(\gamma_p'\) defined above are \((N_x \times N_x),\) in GRMA one defines the number of capture channels, \(N^G(\gamma)^{GRMA}\), as the second dimension of \(\gamma_p'\), namely \(N_g\), the number of levels. Consequently, the original number of \(N_e\) capture channels in \(\gamma_p\) has been reduced to \(N^G(\gamma)^{GRMA}\). Unlike the \(N_e\) true capture channels, these \(N^G(\gamma)^{GRMA}(= N_g)\) GRMA capture channels are composite quantities of many underlying capture channels, and they could be viewed as theoretically motivated formal parameters for improved fitting of cross section data, analogous to capture width parameters of conventional RMA.

A particle-channel width amplitude \((N_x \times N_p)\) matrix \(\gamma_p\) together with \(\gamma_p'\) form a complete \((N_x \times N^G(\gamma)^{GRMA})\) matrix of partial width amplitudes
\[
\gamma_p' = (\gamma_p, \gamma_p'),
\]
where \(N^G(\gamma)^{GRMA} = N_p + N^G(\gamma)^{GRMA}\) and \(N^G(\gamma)^{GRMA} = N_g\). A corresponding GRMA reduced R-matrix can be written in terms of \(\gamma_p'\) as
\[
R = \gamma_p'^T (e - E_1)^{-1} \gamma_p'.
\]
where \(e\) is a diagonal matrix of R-matrix level energies, \(e_{\mu \nu} = E_\mu \delta_{\mu \nu}.\) R-matrix parameters \(e\) and \(\gamma_p'\) could be fitted to cross sections as in SAMMY [6].

\(^1\) It is destructive due to randomly distributed signs of \(\gamma_p\) elements.
For the shift function approximation used here $S_p - B_p = 0$, where $B_p$ is the boundary conditions, the total capture cross section expressed via $(N^y_{\text{GRMA}} \times N^y_{\text{GRMA}}) = (N_i \times N_e)$ matrix $\mathbf{y}'_v$, in Eq. (12) is formally equal to total capture computed via the original $(N_i \times N_e)$ matrix $\mathbf{y}_v$, as shown below. Since $N_y \gg N^y_{\text{GRMA}} = N_i$ for heavy nuclides, this yields a significantly smaller number of parameters that are needed to fit total capture and other cross sections.

The column index of $\mathbf{y}'_v$ matrix labels $N^y_{\text{GRMA}} = N_i$ capture channels that could be thought of as “resonant” capture channels since there is one such capture channel associated with these resonant capture channels could be set to 1, consistent with Eq. (11).

Since the number of channels in GRMA is $N^y_{\text{GRMA}} = N_p + N^y_{\text{GRMA}} = N_p + N_i$, then there would be an advantage, however slight, to using $(N_i \times N_e)$ level-matrix $A$ over the $(N^y_{\text{GRMA}} \times N^y_{\text{GRMA}})$ $R$-matrix in GRMA. However this advantage may not be significant for $N_p \ll N_i$. In contrast to GRMA, $R$-matrix expressions are vastly advantageous over the level matrix in conventional RMA, especially when $N_p \ll N_i$.

Note that a unitary matrix $U$ corresponding to a full $R$-matrix could be divided into blocks introduced before as

$$U \equiv \begin{pmatrix} U_{pp} & U_{pp} \\ U_{pp} & U_{pp} \end{pmatrix}$$

so that a total capture cross section is proportional to (Note that $1_{pp} = 0$)

$$U_{pp}^{(pp)} = \Omega_\gamma P^{(2)/2} y^T \Omega_p^{(2)/2} y_\gamma P^{(2)/2} y_\gamma = \Omega_p P^{(2)/2} y_\gamma A y_\gamma P^{(2)/2} y_\gamma$$

$$\lambda$$

$$= \Omega_p P^{(2)/2} y_\gamma A(\Gamma^{(p)/2}) A y_\gamma P^{(2)/2} y_\gamma$$

$$\lambda$$

since $\Omega_p \Omega_\gamma = 1$, and $L_p = B_p = i P_r$ was assumed on the final line. In that case, total capture is parameterized entirely by $\Gamma^{(p)}$ appearing on the last line of the equation above, and implicitly in the level matrix $A$. Alternatively $R$-matrix could be defined using $y^T$ matrix of partial width amplitudes to be fitted in a standard $R$-matrix formalism. In any case, these identities show that total capture computed by GRMA is formally equal to that of the full $R$-matrix for $S_p = B_p$.

3. Unitarity of (g)RMA

Unitarity of the scattering matrix in GRMA can be established by observing that its reduced $R$-matrix in Eq. (13) is real. Consequently, unitarity of its scattering matrix is guaranteed by the form of the scattering matrix in terms of the $R$-matrix [1].

Preservation of unitarity in the GRMA could be used to justify Fröhner’s prescription that has been conventionally used to enforce unitarity of the total cross section in the conventional RMA [3,6]. For this purpose it is useful to view the conventional RMA as a special case of GRMA in which off-diagonal elements of GRMA capture matrix in Eq. (9) are set to 0 while explicitly retaining the $N^y_{\text{GRMA}} = N_i$ resonant capture channels introduced in Sect. 2. Such an $R$-matrix remains real, and a corresponding scattering matrix (that now includes $N^y_{\text{GRMA}} = N_i$ capture channels) is consequently unitary even for conventional RMA.

Unitarity of the total scattering matrix for conventional RMA justifies Fröhner’s assumption that a total scattering matrix may be assumed unitary. Fröhner used this assumption when deriving the expression for total cross section of conventional RMA, thus enforcing unitarity of the total scattering matrix. A capture cross section was then computed as a difference between the total cross section (computed assuming unitarity) and the total particle-channel cross section computed using conventional RMA particle-channel reduced $R$-matrix.

4. Variance of GRMA matrix elements

Empirical fitting of Reich-Moore capture widths to neutron capture and cross section data using conventional Reich-Moore approximation often reveals variations among RMA capture widths. It is shown below how these empirically observed variations could be used to estimate variance among the off-diagonal elements of $\Gamma^{(p)}$, that are set to 0 in conventional RMA. These considerations may help guide decisions about whether fitting of off-diagonal elements to improve quality of extant fits may be warranted.

An idealized statistical analysis below shows that the variance of diagonal elements in $\Gamma^{(p)}$ is approximately two times larger than the variance of its off-diagonal elements. Capture widths fitted using a conventional RMA are expected to deviate slightly from the diagonal values of full $\Gamma^{(p)}$ because in the process of fitting their values could compensate for missing diagonal elements omitted in conventional RMA. Assuming that variance of conventional RMA capture widths approximately equals variance of diagonal elements of $\Gamma^{(p)}$, their large variance would indicate a large variance among off-diagonal elements, and this may suggest that fitting of off-diagonal elements could improve the overall fit.

Diagonal elements of $\Gamma^{(p)}$ are $\chi^2$-distributed with $N_v$ degrees of freedom when elements of $y_\gamma$ are approximated by a symmetric normal distribution of variance $\sigma_0^2$. In this case, a mean of diagonal elements is $\langle \Gamma^{(p)} \rangle = \sigma_0^2 N_v$, and their variance is $\text{Var}(\Gamma^{(p)}) = 2\sigma_0^2 N_v = 2(\Gamma^{(p)})^2 / N_v$. Its off-diagonal elements obey a variance-gamma distribution [12]. Assuming no correlation among partial capture widths, it has a mean 0 and variance $\text{Var}(\Gamma^{(p)}) = \sigma_0^2 N_v = \text{Var}(\Gamma^{(p)})/2$. Consequently, a large variance among capture widths of a conventional RMA implies that magnitudes of some of the neglected off-diagonal elements would be comparable (to the square root of) half of the variance of the conventional RMA capture widths. Figures 1 and 2 show that variation among conventional RMA capture widths are tangible.

The number of $\gamma$-ray channels, or the number of degrees of freedom, increases with resonance energy as new capture channels into levels open up below. Due to large variation among amplitudes associated with different multipolarities, normal distributions of vastly different magnitudes contribute to the same matrix element. Consequently, it is likely that a subset of strongest $\gamma$-ray transitions, i.e. electric dipole ($L = 1$) transitions, may determine the number of effective degrees of freedom of the $\chi^2$ distribution of a given matrix element.
This may reduce the effective number of degrees of freedom and thus increase the overall variance. Although Wishart distribution should therefore be viewed as an approximation, it may yield useful information about marginal statistics of diagonal and off-diagonal elements of capture width matrix $\gamma'$. Departure from idealized statistics may indicate presence of underlying doorway states that would require special treatment.

5. Alternative GRMA parameters

An alternative $R$-matrix parameterization equivalent to formal $R$-matrix parametrization has been derived in Ref. [9]. This section describes how the Brune transform between formal and alternative $R$-matrix parameters derived in Ref. [9] can be directly applied to GRMA $R$-matrix parameters and by specialization to those of conventional RMA. To this end, it is sufficient to observe that Brune transform depends on shift-functions and boundary conditions constants of all channels considered. In this work, shift functions and boundary conditions of $\gamma$-ray channels in GRMA have been approximated by $S_\gamma - B_\gamma = 0$. Therefore, Brune transform will be unaffected by inclusion of such $\gamma$-ray channels. Consequently, the matrices governing conversion between alternative and formal $R$-matrix partial width amplitudes are to be computed as if $\gamma$-ray channels were absent. These conversion matrices are to be applied to particle and to GRMA $\gamma$-ray widths alike: GRMA capture width amplitudes matrix $\gamma'_\gamma$ is to be transformed just like that of particle-channel partial widths amplitudes, that is,

$$\tilde{\gamma}'_{\gamma'} = a^T \gamma'_{\gamma'}.$$  \hspace{1cm} (17)

This implies that transformation of conventional RMA capture widths of a diagonal $\gamma'_{\gamma'}$ matrix would yield $\tilde{\gamma}'_{\gamma'}$ with finite off-diagonal elements. This demonstrates that GRMA is necessary to maintain equivalence between formal and alternative $R$-matrix parameterizations.

One useful property of Brune’s alternative $R$-matrix, $\tilde{R}$ in notation of Ref. [9], is that it effectively satisfies energy-dependent boundary condition $S(E) - B = 0$. Application of this boundary condition into the expression for the scattering matrix $U$ in terms of $\tilde{R}$ yields an elegant expression for a (real and symmetric) $K$-matrix

$$K = P^{1/2} R P^{1/2},$$  \hspace{1cm} (18)

where $\tilde{R}$ is the alternative $R$-matrix derived by Brune.

6. Conclusions and outlook

Generalized Reich-Moore approximation (GRMA) provides some formal advantages and a new perspective over the conventional Reich-Moore approximation (RMA). The manifest unitarity of GRMA made the unitarity of conventional RMA more apparent. Furthermore, it was shown how GRMA $R$-matrix parameters could be naturally converted between formal and alternative $R$-matrix parameters [9]. Unlike the conventional RMA, GRMA can formally reproduce the total capture cross sections, so it may yield improved fits to measured cross sections at the cost of introducing additional capture width amplitudes. The magnitude of any such improvements will be quantified in a future publication.

7. Appendix

Summary of the notation used in the paper:

- $N_c = \#$ of $R$-matrix levels
- $N_p = \#$ of particle channels
- $N_\gamma = \#$ of $\gamma$-ray (i.e., radiative capture) channels
- $N_c = \#$ of all channels in full $R$-matrix
- $N_c = N_p + N_\gamma$ in full $R$-matrix
- $N_{GRMA} = \#$ of all channels in GRMA $R$-matrix
- $N_{GRMA} = \#$ of GRMA $\gamma$-ray channels
- $N_{GRMA} = N_p + N_{GRMA}^\gamma$ in GRMA $R$-matrix
- $N_{GRMA}^\gamma = N_\gamma$, as argued below Eq. (11)
One of the key results of this work, namely $N^{\text{GRMA}}_{\gamma} = N_{\lambda}$, thus equates the number of $R$-matrix levels, $N_{\lambda}$, to the number of GRMA capture channels, $N^{\text{GRMA}}_{\gamma}$.

Useful and motivating discussions with Carl Brune, Ian Thompson, Gerry Hale, Mark Paris, and James deBoer are gratefully acknowledged. This work was supported by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for DOE.

References

[1] A.M. Lane and R.G. Thomas, Rev. Mod. Phys. 30, 257 (1958)
[2] F. Gunsing, Proceedings of Ecole Joliot Curie (EJC2014), https://ejc2014.sciencesconf.org
[3] F. Fröhner, JEFF Report 18 (2000)
[4] D. Baye and P. Descouvemont, Scholarpedia 8(1), 12360 (2013)
[5] National Nuclear Data Center, Brookhaven National Laboratory, http://nndc.bnl.gov
[6] N.M. Larson, ORNL/TM-9179/R8 (2008)
[7] M.T. Pigni, C. Gauld, and S. Croft, Proceedings of the International Conference on Nuclear Data for Science and Technology (ND2016), Brugge, Belgium, September 11–16, 2016
[8] C.W. Reich and M.S. Moore, Phys. Rev. 111, 929 (1958)
[9] C. Brune, Phys. Rev. C66, 044611 (2002)
[10] R.E. Azuma, et al., Phys. Rev. C50, 1194 (1994)
[11] A. Bohr and B. Mottelson, Nuclear Structure, Vol. 1, Section 3C-2, W.A. Benjamin, Inc. (1969)
[12] J. Wishart, Biometrika 20A(1–2), 32 (1928); https://en.wikipedia.org/wiki/Wishart_distribution
[13] M.T. Pigni and L.C. Leal, Proceedings of the International Conference on Nuclear Criticality Safety (ICNC 2015), Charlotte, NC, September 130–17, 2015
[14] M.T. Pigni, G. Žerovnik, L.C. Leal, and A. Trkov, Proceedings of the International Conference on Nuclear Data for Science and Technology (ND2016), Brugge, Belgium, September 11–16, 2016