

Effective R-Matrix Parameterizations for Nuclear Data*

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Abstract. We derive an effective Reich-Moore approximation (RMA) of the Wigner-Eisenbud R -matrix formalism parameterized by complex-valued resonance energies and widths; this RMA exactly reproduces the total eliminated cross section. We show that resonance parameters evaluated for a conventional boundary conditions (BCs), $B_c = S_c(E)$,*** are approximately equal to the R -matrix parameters in Park's formalism by employing a linear approximation of the shift function therein [T.-S. Park, Phys. Rev. C **106** (2021) 064612]. We outline a method for converting Park's observed reduced width amplitudes (RWAs) and their covariance matrix into Brune's alternative R -matrix RWAs and their covariance matrix [C. Brune, Phys. Rev. C **66** (2002) 044611]. We extend the Park's R -matrix formalism into the complex plane by introducing a complex-valued basis set of eigenfunctions of a complex-symmetric (non-Hermitian) Hamiltonian in the R -matrix interior. We observe that its R -matrix resonance energies and widths are directly related to the poles and residues, respectively, of Hwang's sum-over-poles representation of cross sections [R.N. Hwang, Nucl. Sci. Eng. **96** (1987) 192].

1 Introduction

Statistical assumptions or approximations used in resolved resonance data evaluations based on the R -matrix are being reviewed in the context of evaluations performed under the auspices of the International Nuclear Data Evaluation Network Light Elements (INDEN-LE) [4]. To contribute to these efforts, we show analytically how the conventional Reich-Moore approximation (RMA), in which resonance energies alone are complex-valued, can be improved by introducing complex-valued widths. We also show that it yields the total cross section of eliminated capture channels exactly as it would if computed from the exact R -matrix. We also consider applications of the effective RMA toward elimination of other kinds of channels.

Additionally, the INDEN-LE collaboration has scrutinized a conventional choice for BCs, specifically $B_c = S_c(E)$, which is commonly used for resolved resonance cross section data

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***The R -matrix boundary conditions and the shift function, $S_c(E)$, are discussed in, e.g., [1–3].

evaluations performed by the SAMMY code [2] and was adopted by the US Evaluated Nuclear Data File (ENDF) [5]. These BCs have been used extensively by Lane and Thomas in their review article [1] to simplify some analytical derivations. We will use the R -matrix formalism recently derived by Tae-Sun Park [6] to clarify the implications of this choice of BC and to describe why this choice has been useful despite its deviation from the R -matrix formalism, however slight. In particular, we show that the Park's R -matrix parameters coincide with those of the $B_c=S_c(E)$ BC when adopting a linear approximation for slowly varying shift functions that appear in the R -matrix of Park.¹

To transform the latter parameter set to that of the Wigner-Eisenbud's, all that remains is to transform Park's resonance parameters to those of Brune's alternative R -matrix because the transformation between the Brune's and the Wigner-Eisenbud's parameters has already been derived [7]. The transformation of Park's observed reduced width amplitudes (RWAs) to Brune's alternative RWAs is described in Section 2.3, whereas the observed resonance energies of Park and Brune are known to be equal [6]. The R -matrix formalisms, parameterizations, and transformations just mentioned are represented by boxes and arrows in a more general schema in Figure 1.

One practical advantage of the R -matrix formalism parameterized by the observed resonance energies (corresponding to locations of the observed peaks in a given cross section) is that it simplifies refining of the energy-mesh around the peaks on which the cross section is computed during an evaluation. This is in contrast to the formal R -matrix resonance energies which are shifted relative to the peaks for orbital angular momentum quantum number, l , greater than zero. There is a similar advantage to having a formalism parameterized by the observed RWAs because they are directly related to the widths of the observed resonance peaks.

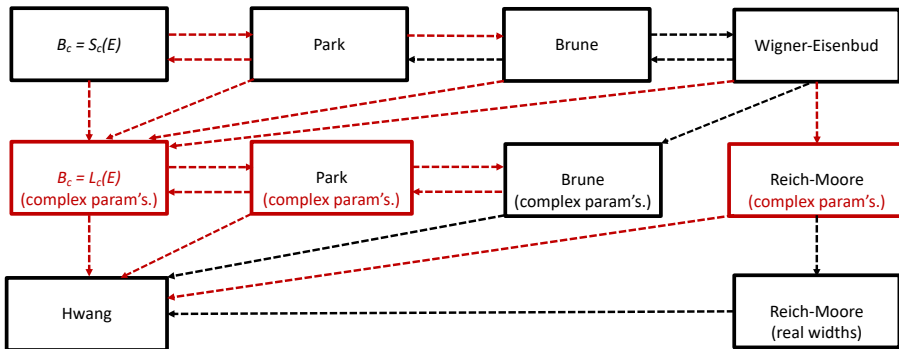


Figure 1. Phenomenological R -matrix formalisms considered in this work are represented by their respective boxes, and some transformations among their parameter sets are represented by arrows. Red lines or text indicates a formalism or transformation introduced in this work. Black lines or text indicates an extant formalism or parameter transformations.

2 Formal derivations

In Section 2.1, we start from a general expression for the reduced R -matrix derived by Lane and Thomas (LT) [1] to derive an effective RMA with complex-valued resonance energies and widths and to show that it exactly reproduces the total eliminated cross section. In Section 2.2, we use the perspective provided by the Park's R -matrix formalism [6] to improve

¹ Assuming sufficient accuracy of the linear approximation, we treat the Park's resonance parameters as approximately equal to those evaluated using the $B_c=S_c(E)$ BC.

our understanding of the conventional $B_c = S_c(E)$ BC [2]. In Section 2.3, we describe an algorithm for converting the observed RWA R -matrix parameters of Park to Brune's alternative R -matrix RWAs. In Section 2.4, we extend Park's formalism into the complex plane, in which (complex-valued) resonance energies conveniently correspond to the poles of the scattering matrix in the complex plane.

2.1 Transforming the reduced R -matrix of LT to an effective RMA

To improve the RMA, we start with a general analytical expression for the reduced R -matrix found in Eqs. (X.1.7-9a) of LT [1], where a reduced R -matrix is given as

$$\mathcal{R} = \gamma_r^\top A^{-1} \gamma_r \quad (1)$$

$$= \gamma_r^\top [\mathbf{e} - \xi - E\mathbf{1}]^{-1} \gamma_r, \quad (2)$$

where² \mathbf{e} is a diagonal matrix of Wigner-Eisenbud's formal resonance energy parameters,

$$\xi \equiv \gamma_e L'_e \gamma_e^\top, \quad (3)$$

is a symmetric matrix, and where, by using the notation of LT [1], we have set $L'_e = L_e^0 \equiv L_e - B_e$ and $R_{ee}^0 = 0$.³ Being analytically exact, these expressions reproduce the total and the total eliminated cross section⁴ that would be computed from the exact prior R -matrix. Consequently, preservation of analytical equivalence with the expression above ensures that the total and the total eliminated cross section are preserved exactly.

To show how an *effective* set of reduced R -matrix parameters may become complex-valued, an eigenvalue decomposition (EVD) of a *symmetric*⁵ matrix $\mathbf{e} - \xi$ is assumed to exist:

$$\mathbf{e} - \xi = \mathbf{v} \mathbf{\epsilon} \mathbf{v}^\top, \quad (4)$$

where $\mathbf{v} \mathbf{v}^\top = \mathbf{1}$ and $\mathbf{\epsilon}$ is diagonal. Using this EVD in Eq. (2) yields an equivalent expression for the reduced R -matrix of LT:

$$\mathcal{R} = \gamma_r^\top [\mathbf{v} \mathbf{\epsilon} \mathbf{v}^\top - E\mathbf{1}]^{-1} \gamma_r, \quad (5)$$

$$= \gamma_r^\top [\mathbf{v} (\mathbf{\epsilon} - E\mathbf{1}) \mathbf{v}^\top]^{-1} \gamma_r, \quad (6)$$

$$= \gamma_r^\top (\mathbf{v}^\top)^{-1} [\mathbf{\epsilon} - E\mathbf{1}]^{-1} \mathbf{v}^{-1} \gamma_r, \quad (7)$$

$$= (\gamma_r^\top \mathbf{v}) [\mathbf{\epsilon} - E\mathbf{1}]^{-1} (\mathbf{v}^\top \gamma_r), \text{ and} \quad (8)$$

$$= \mathbf{g}_r^\top [\mathbf{\epsilon} - E\mathbf{1}]^{-1} \mathbf{g}_r, \quad (9)$$

where $\mathbf{g}_r \equiv \mathbf{v}^\top \gamma_r$ and $(\mathbf{\epsilon}, \mathbf{g}_r)$ may be viewed as an *effective* reduced R -matrix parameter set that could be optimized independently of the formal parameter set $(\mathbf{e}, \gamma_r, \gamma_e)$.

For L_e independent of energy, E , as is assumed for capture channels for which $L_{\gamma_e} = i\mathbf{P}_{\gamma_e} = i$, matrix ξ is symmetric⁶ and complex-valued, the effective reduced R -matrix parameters are complex-valued and independent of energy, thus maintaining the advantage of energy-independent R -matrix parameters. A conventional RMA implemented in SAMMY is recovered for a (real-valued) diagonal \mathbf{e} and a pure imaginary-valued *diagonal* ξ , for which $\mathbf{v} = \mathbf{1}$, $\mathbf{\epsilon} = \mathbf{e} - \xi$, and $\mathbf{g}_r = \gamma_r$.

²Labels r and e refer to *retained* and *eliminated* subsets of channels, respectively.

³The prime symbol in L'_e is copied verbatim from LT [1] and does not represent a derivative in this instance.

⁴The total eliminated cross section is a measure of deviation of the scattering matrix from unitarity caused by the imaginary components of $(\mathbf{\epsilon}, \mathbf{g}_r)$.

⁵The same form of EVD holds for complex-valued symmetric matrix, for which \mathbf{v} and $\mathbf{\epsilon}$ may be complex-valued.

⁶Its dominant elements lie along its diagonal, where they are the sum of squares of RWAs of eliminated channels for each resonance; off-diagonal elements are expected to be much smaller due to expected random distribution of (complex) phases among the RWAs of eliminated capture channels for *distinct* resonances.

On the other hand, for L_e energy-dependent (whether real- or complex-valued), the eigenvector matrix \mathbf{v} , and hence the matrix of effective RWAs (\mathbf{g}_r), is also energy dependent, thereby shedding the advantage of having energy-independent R -matrix parameters.⁷

2.2 A Perspective on the $B_c = S_c(E)$ BC from Park's R -matrix formalism

Park's R -matrix formalism and its energy dependence in terms of observed resonance energies and RWAs in particular, provide a useful vantage point to interpret the $B_c = S_c(E)$ approximation employed by the SAMMY code [2]. For completeness, we render the R -matrix derived by Park as

$$\mathbf{R}_S^{(\text{Park})} = \boldsymbol{\gamma}^\top (\mathbf{e} - S(E) - E\mathbb{1})^{-1} \boldsymbol{\gamma}. \quad (10)$$

The subscript S is introduced to distinguish it from the complex-valued matrix, $\mathbf{R}_L^{(\text{Park})}$, introduced in Eq. (22). Here, $\mathbf{e} = \text{diag}(\{E_\lambda\})$ is a diagonal matrix of observed (real-valued) resonance energies, where

$$[S(E)]_{\lambda\lambda'} = \begin{cases} \sum_c \gamma_{\lambda c}^2 [S_c(E) - S_{\lambda c} + (E_\lambda - E)S'_{\lambda c}], & \text{for } \lambda' = \lambda, \\ \sum_c \gamma_{\lambda c} \gamma_{\lambda' c} \left[S_c(E) + \frac{(E_{\lambda'} - E)S_{\lambda c} - (E_\lambda - E)S_{\lambda' c}}{E_\lambda - E_{\lambda'}} \right], & \text{for } \lambda' \neq \lambda, \end{cases} \quad (11)$$

with $S_{\lambda c} \equiv S_c(E_\lambda)$ and $S'_{\lambda c} \equiv \left. \frac{dS_c(E)}{dE} \right|_{E=E_\lambda}$ (see Eq. (29) of [6]). Inserting a linear approximation⁸ for the shift function around a level, E_λ , specifically,

$$S_c(E) = S_{\lambda c} - (E_\lambda - E)S'_{\lambda c} \quad (12)$$

into a corresponding diagonal element of $S(E)$ in Eq. (11) makes it equal to 0. Analogously, a linear approximation for the shift function that appears in the off-diagonal elements of $[S(E)]_{\lambda\lambda'}$ (i.e., a linear interpolation between points $(E_\lambda, S_{\lambda c})$ and $(E_{\lambda'}, S_{\lambda' c})$) makes each of the off-diagonal elements vanish. Because the entire matrix $S(E)$ is made to vanish for this linear approximation, the R -matrix parameterization in Eq. (10) attains a form identical to that for the $B_c = S_c(E)$ BC. Consequently, the resonance parameters evaluated for the $B_c = S_c(E)$ BC can be thought of as the observed resonance parameters in Park's formalism (when using the linear approximation just described) and have been interpreted as such in the SAMMY code [2].

2.3 Transforming observed RWAs into Brune's alternative RWAs

Because of its relatively recent introduction to the nuclear data evaluation community [4], there is some interest in transforming the observed R -matrix parameter sets of the Park's R -matrix formalism [6] to their equivalent sets in the Wigner-Eisenbud's R -matrix formalism [1] or its alternative parameterization derived by Brune [7]. Because the transformation between the Wigner-Eisenbud's and Brune's alternative R -matrix parameterization has been published, it will suffice to describe the conversion between the parameterizations of Park

⁷One may choose to neglect such energy dependence when its effect is not appreciable.

⁸According to the plot of $S_l(E)$ in Fig. 3.a of [3], where an analytical continuation was used for $E < 0$, a linear approximation is expected to be accurate for all *even* orbital angular momenta, " l ", and for all *odd* values of l (with a possible exception for $l = 1$, which would need to be scrutinized) in the energy range covered in evaluations based on R -matrix formalism; whether this approximation is sufficiently accurate could be ascertained by comparing evaluations that use the exact formalism of Park.

and Brune. As explained by Park [6], the observed resonance energies coincide with the alternative resonance energies of Brune, and the observed RWAs relate to the alternative RWAs of Brune via Eq. (34) of [6], as restated here for completeness:⁹

$$\gamma_{\lambda c}^{\text{obs}} = \tilde{\gamma}_{\lambda c} [1 + \sum_{c'} \tilde{\gamma}_{\lambda c'}^2 S'_{\lambda c'}]^{-1/2}, \quad (13)$$

where $\tilde{\gamma}_{\lambda c}$ are the alternative RWAs defined by Brune [7]. Transforming from Brune's alternative RWAs to Park's observed RWAs amounts to evaluating the right hand side of this expression, whereas the inverse transform can be achieved by applying the Newton-Raphson method. For the sake of inverting this expression by the Newton-Raphson method, we convert it to linear algebra form¹⁰,

$$\mathbf{f}(\mathbf{x}) = \mathbf{x}(1 + \mathbf{x}^\top \mathbf{S}' \mathbf{x})^{-\frac{1}{2}}, \quad (14)$$

where \mathbf{x} is a channel vector of formal RWAs, $\tilde{\gamma}_{\lambda c}$, for a fixed resonance, λ , where \mathbf{S}' is a diagonal channel matrix of shift function derivatives evaluated at the observed resonance energy, and where, for convenience, we define

$$\chi^2(\mathbf{x}) \equiv (\langle \mathbf{y} \rangle - \mathbf{f}(\mathbf{x}))^\top \mathbf{Y}^{-1} (\langle \mathbf{y} \rangle - \mathbf{f}(\mathbf{x})) \quad (15)$$

Here, $\langle \mathbf{y} \rangle$ represents a channel vector of (the expectation values¹¹ of) observed RWAs, $\gamma_{\lambda c}^{\text{obs}}$, of the same level, λ , so that $\chi^2(\mathbf{x})$ can be minimized independently for each level by a Newton-Raphson method, and where

$$\mathbf{Y} \equiv \langle (\mathbf{y} - \langle \mathbf{y} \rangle)(\mathbf{y} - \langle \mathbf{y} \rangle)^\top \rangle \quad (16)$$

is a covariance matrix of Brune's alternative RWAs. This covariance matrix would be needed to obtain its posterior covariance matrix, \mathbf{X}' , which is a Hessian of $\chi^2(\mathbf{x})$ evaluated at $\langle \mathbf{x} \rangle'$. From a Bayesian perspective, the expression for the $\chi^2(\mathbf{x})$ in Eq. (15) assumes that the data, represented by $\langle \mathbf{y} \rangle$ and \mathbf{Y} , and the model, given by Eq. (14), are perfect. It also assumes that all probability distribution functions are normal (i.e., Gaussian) and that the model is linear or that it can be approximated linearly. These assumptions, although imposing strong constraints on the solution, are not expected to introduce a significant aberration from a true solution, $\langle \mathbf{x} \rangle'$; however, imposition of these assumptions may yield a covariance matrix, \mathbf{X}' , which underestimates the true uncertainties of $\langle \mathbf{x} \rangle'$. Minimization of $\chi^2(\mathbf{x})$ by an iterative Newton-Raphson method yields a solution when $\chi^2(\mathbf{x}) = 0$ is reached; converting the solution and its covariance ($\langle \mathbf{x} \rangle'$ and \mathbf{X}' , respectively) back to the observed RWAs of Park via Eq. (13), and comparing to the original (i.e. prior) observed RWAs of Park and its covariance ($\langle \mathbf{y} \rangle$ and \mathbf{Y} , respectively), could quantify any error that may have been incurred by the transformation.¹²

2.4 Extension of Park's R -matrix formalism into complex plane

Inspired by Park's derivation [6], we adapt it to complex-symmetric,¹³ non-Hermitian Hamiltonian operators, \mathcal{H} , whose bi-orthogonal basis set of eigenfunctions of decaying compound

⁹Squaring this expression is equivalent to Eq. (16) of Brune [7].

¹⁰The existence of an analytical solution to the inverse transform, $\mathbf{x} = \mathbf{f}(\mathbf{x})(1 - \mathbf{f}(\mathbf{x})^\top \mathbf{S}' \mathbf{f}(\mathbf{x}))^{-\frac{1}{2}}$, appearing in Eq. (42) of [8] has been kindly brought to our attention by Ian J. Thompson after the submission of this manuscript.

¹¹Expectation values are implied by the angled brackets, $\langle \cdot \rangle$.

¹²This transformation method could be generalized further by utilizing the concept of generalized data, $\boldsymbol{\zeta} \equiv (\mathbf{x}, \mathbf{y})$, and of generalized parameters, $\mathbf{z}(\mathbf{x}) \equiv (\mathbf{x}, \mathbf{f}(\mathbf{x}))$, with which the cost function becomes $\chi^2(\mathbf{x}) = (\langle \boldsymbol{\zeta} \rangle - \mathbf{z}(\mathbf{x}))^\top \mathbf{C}^{-1} (\langle \boldsymbol{\zeta} \rangle - \mathbf{z}(\mathbf{x}))$, where \mathbf{C} is a covariance matrix of \mathbf{z} , which could be minimized [9, 10].

¹³For a complex-symmetric matrix acting to its left, as in Eq. 18, Hermitian conjugation is not needed.

nuclear resonant states within the R -matrix channel radius can be defined as

$$\mathcal{H}|\mathcal{X}_\lambda\rangle = \mathcal{E}_\lambda|\mathcal{X}_\lambda\rangle \quad \text{and} \quad (17)$$

$$\langle\mathcal{X}_\lambda|\mathcal{H} = \langle\mathcal{X}_\lambda|\mathcal{E}_\lambda, \quad (18)$$

where $|\mathcal{X}_\lambda\rangle$ and $\langle\mathcal{X}_\lambda|$ are (complex-valued) vector-transposes of each other (with complex-valued discrete eigenvalue spectrum $\{\mathcal{E}_\lambda\}$), thereby satisfying the following orthonormality¹⁴ relation:

$$\langle\mathcal{X}_\lambda|\mathcal{X}_{\lambda'}\rangle = \int \mathcal{X}_\lambda \mathcal{X}_{\lambda'} d\tau = \delta_{\lambda\lambda'}. \quad (19)$$

Here, the integration is over the volume of the interior region but without the complex conjugation of \mathcal{X}_λ appearing in Eq. (7) from Park [6] for Hermitian Hamiltonians [11, 12]. The orthonormality relation in Eq. (19) can be stated in terms of complex-valued radial functions,

$$\sum_c \int_0^{a_c} dr_c \mathcal{U}_{\lambda c}(r_c) \mathcal{U}_{\lambda' c}(r_c) = \delta_{\lambda\lambda'}, \quad (20)$$

without the complex conjugation of $\mathcal{U}_{\lambda c}(r_c)$.

With the distinctions introduced above, the formal steps of Park's derivation in Eqs. (8–29) [6] can be retraced step-by-step for a corresponding overlap matrix:

$$\mathcal{J}_{\lambda\lambda'} \equiv \int \mathcal{X}_\lambda \mathcal{X}_{\lambda'} d\tau. \quad (21)$$

All the steps in the original derivation of the of the R -matrix by Park [6] can be retraced for the complex basis introduced above to yield a corresponding form in which resonance parameters are replaced by their complex-valued counterparts, $\{\mathcal{E}_\lambda, \gamma_{\lambda c}\}$, and any appearance of the shift function, $S_c(\cdot)$, is analogously replaced by a complex-valued logarithmic derivative,¹⁵ $L_c(\cdot)$, to yield¹⁶

$$\mathbf{R}_L^{(\text{Park})} = \boldsymbol{\gamma}^\top (\boldsymbol{\varepsilon} - \mathcal{L}(E) - E\mathbb{1})^{-1} \boldsymbol{\gamma}, \quad \text{where} \quad E, [\boldsymbol{\gamma}]_{\lambda c} \in \mathbb{C}, \quad (22)$$

and $\boldsymbol{\varepsilon} = \text{diag}(\{\mathcal{E}_\lambda\})$ is a diagonal matrix of observed *complex*-valued resonance energies, \mathcal{E}_λ , where

$$[\mathcal{L}(E)]_{\lambda\lambda'} = \begin{cases} \sum_c \gamma_{\lambda c}^2 \left[L_c(E) - L_{\lambda c} + (\mathcal{E}_\lambda - E)L'_{\lambda c} \right], & \text{for } \lambda' = \lambda, \\ \sum_c \gamma_{\lambda c} \gamma_{\lambda' c} \left[L_c(E) + \frac{(\mathcal{E}_{\lambda'} - E)L_{\lambda c} - (\mathcal{E}_\lambda - E)L_{\lambda' c}}{\mathcal{E}_\lambda - \mathcal{E}_{\lambda'}} \right], & \text{for } \lambda' \neq \lambda. \end{cases} \quad (23)$$

Here, $L_{\lambda c} \equiv L_c(\mathcal{E}_\lambda)$, and the observed designations of complex-valued resonance energies and RWAs refer to poles and residues of the cross section in the complex plane. Following the logic outlined in Section 2.2, a linear approximation¹⁷ of $L_{\lambda c}(E)$ around \mathcal{E}_λ makes each element of the $\mathcal{L}(E)$ matrix vanish to yield a sum-over-poles representation of the scattering matrix, where pole positions are defined by $\{\mathcal{E}_\lambda\}$, and the residues are defined via the matrix of RWAs, $\boldsymbol{\gamma}$. Notably, the poles and the residues of the scattering matrix can be found from various R -matrix parameterizations (Wigner-Eisenbud RMA, Brune, or Park) by numerically finding the poles and residues of the corresponding scattering matrix [13–15].

¹⁴This orthonormality is analogous to that between the left and right eigenvector matrices, $\boldsymbol{v}\boldsymbol{v}^\top = \mathbb{1}$, of a complex-symmetric matrix $\boldsymbol{\xi}$ considered in Section 2.1.

¹⁵For example, $B_{\lambda c} = S_c(E_\lambda)$ is replaced by $B_{\lambda c} = L_c(\mathcal{E}_\lambda)$.

¹⁶The quantity in parenthesis corresponds to the complex-valued A -matrix of Park [6].

¹⁷Plots of the shift, $S_c(E)$, and the penetrability function, $P_c(E)$, in Figure 3 of [3] show that a linear approximation of $L_c(E) \equiv S_c(E) + iP_c(E)$ is likely accurate; a possible exception for the $c = l = 1$ case ought to be scrutinized.

3 Concluding remarks

We presented several lesser-known connections among various R -matrix formalisms and parameterizations, described methods for transforming among their respective parameter sets, and outlined a method for corresponding transformations of covariance matrices. Park's R -matrix formalism was used to link the $B_c = S_c(E)$ BC parameters to Brune's alternative R -matrix parameters and from those to the Wigner-Eisenbud parameters. Properties of complex-symmetric Hamiltonian matrices and their eigenvalues and eigenvectors were used to derive (1) an effective RMA parameterized by complex-valued energies *and* widths to reproduce the total cross section of the eliminated channels and (2) a complex-plane analogue of Park's R -matrix formalism to provide a direct connection from the complex-valued resonance energies and RWAs to the poles and residues, respectively, of the scattering matrix [13, 15]. We hope that some of the effective R -matrix parameterizations introduced here, and the transformations among them, may lead to improvements in R -matrix evaluation codes [2, 16], the quality of evaluated nuclear data libraries [5], and the fidelity of neutron transport simulations for the Nuclear Criticality Safety Program and nuclear engineering.

4 Acknowledgments

Useful discussions with Helmut Leeb, Ian J. Thompson, Mark W. Paris, Gerald M. Hale, Zhenpeng Chen, and other INDEN-LE Meeting participants are gratefully acknowledged.

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the US Department of Energy.

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