Definite complete invariant parametrization of *R*-matrix theory

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We establish a definite parametrization of *R*-matrix theory, which is complete and invariant. Compared to the traditional parametrization of Wigner and Eisenbud, our parametrization has the major advantage of having no arbitrary boundary condition B_c, and of being constituted of scattering matrix poles $\mathcal{E}_\lambda$, which are physical quantities and hence invariant with the choice of arbitrary channel radii a_c. Moreover, being the poles of the scattering matrix, the definite levels $\mathcal{E}_\lambda$ correspond exactly to the nuclear resonances. Our definite parametrization is also global and complete, meaning a finite number of definite parameters—the same number as the Wigner and Eisenbud ones, minus the boundary conditions—can fully describe the scattering matrix on the whole complex plane [it is thus not a local description restricted to an energy window as the previous Windowed Multipole Representation of Ducru *et al.*, Phys. Rev. C **103**, 064610 (2021)]. These benefits come at the cost of requiring all parameters to now be complex numbers without an explicit set of constraints, which significantly complicates their direct nuclear data evaluation. We show that our parametrization also gives rise to shadow poles, though we prove they can be ignored and still completely reconstruct the scattering matrix with all its poles, and thus describe nuclear cross sections exactly. This means our parametrization only requires as many scattering matrix poles $\mathcal{E}_\lambda$ as there are Wigner-Eisenbud resonance levels E_λ, thereby establishing a one-to-one correspondence between the traditional Wigner-Eisenbud and our definite parametrization of *R*-matrix theory. Remarkably, we show these same cross sections can also be obtained using the shadow poles instead of the principal poles. We observe evidence of these phenomena in the spin-parity group $J^\pi = 1/2^{(-)}$ of xenon isotope ^{134}Xe.

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I. INTRODUCTION

When two bodies collide and interact, several outcomes are possible, and cross sections quantify the relative likelihood that any one of these outcomes occurs. As such, cross sections are a central pillar of our collective nuclear physics knowledge.

Since nuclear cross sections vary with the energy and momentum of the collision, a convenient and compact way to describe this energy dependence is desirable in order to document all these nuclear reactions.

R-matrix theory—a two-body-in–two-body-out quantum model of nuclear interactions—has provided such convenient means for documentation, by establishing a set of *resonance parameters* which can fully characterize nuclear cross sections [1–4].

Our knowledge of nuclear cross sections is thus captured in the form of these resonance parameters, fitted from an extensive body of experimental measurements (evaluation process), and compiled into our standard evaluated nuclear data libraries (ENDF [5], JEFF [6], BROND [7], JENDL [8], CENDL [9], TENDL [10,11]).

These nuclear data libraries are all based on traditional *Wigner-Eisenbud R*-matrix resonance parameters, which have many advantages, chief amongst which is the fact that these parameters are real numbers with explicit constraints, greatly simplifying both their evaluation and the format with which they are reported. Perhaps the major drawback of the Wigner-Eisenbud parametrization of *R*-matrix theory is that it requires prescribing two arbitrary parameters: the boundary conditions B_c and the channel radii a_c. This means that, from the same experimental data, carrying out two evaluations with different prescriptions of arbitrary parameters will yield different resonance parameter values, even though they are describing the same physical cross section. Moreover, there is no simple way of converting the resonance parameters obtained from one arbitrary prescription to another.

To address this problem, physicists have proposed alternative ways of parametrizing cross sections, based on the same *R*-matrix model of nuclear interactions, hoping to constitute new improved nuclear data libraries.

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One such alternative parametrization was proposed by Brune in [12] (building on Barker's work [13]), and we established new properties of this parametrization and generalized it to the Reich-Moore formalism in [14]. Originally, the Brune parametrization had the major advantage of being constituted of real parameters that are independent of the arbitrary boundary condition B_c, thus removing the need to specify any arbitrary boundary condition B_c at all. Also, the Brune alternative resonance energies are closer to the resonances than the traditional Wigner-Eisenbud resonance energies. These two advantages have led some people to adopt the Brune parametrization for evaluations of light nuclides [15].

And yet, the Brune parameters also have drawbacks. They are all dependent on the arbitrary choice of channel radii a_c. Moreover, we also showed that when generalizing the Brune parametrization to the Reich-Moore formalism (of great practical importance for heavy nuclides [16]), the Brune parameters become complex, and suffer from several complications [14]. Furthermore, though close to them, the Brune alternative resonance energies do not correspond exactly to the resonances.

This is because the natural physical quantities describing the resonances of the interaction are the poles $\mathcal{E}_\lambda$ of the scattering matrix, which is why an entire field has been dedicated to pole expansions of nuclear reactions (Humblet and Rosenfeld theory of nuclear reactions [17–25], and general mathematical theory of scattering processes [26]). While the bridge between R-matrix theory and pole expansions was recently established in the windowed multipole representation of R-matrix cross sections [27,28], the major drawback of pole expansions is that there are in general an infinity of poles $\mathcal{E}_\lambda$ to the scattering matrix. Even in the case of a finite number of poles, there are no explicit formulas for the nonresonant background contributions (holomorphic part of the scattering matrix Mittag-Leffler expansion). Pole expansions are therefore bound to be local parametrizations: limited to approximating the scattering matrix in a certain energy region (this is the essence of the windowed multipole representation [27]).

R-matrix theory, and in particular the Wigner-Eisenbud parameters, were introduced for calculability reasons: to establish a global parametrization encompassing the entire energy range, and completely describe the scattering matrix with a small number of parameters.

In this article, after recalling the Wigner-Eisenbud parametrization in Sec. II, we establish in Sec. III a new definite, complete, invariant parametrization of R-matrix theory.

By completely parametrizing the scattering matrix using only as many of its poles $\mathcal{E}_\lambda$ as there are Wigner-Eisenbud resonance levels E_λ (that is N_λ levels), our definite parametrization seeks to combine the best aspects of both natural pole expansions and R-matrix complete parametrizations. Our definite parametrization is complete and global (requiring neither local expansions nor approximations), with a one-to-one correspondence to the traditional Wigner-Eisenbud resonance parameters. Not only does our parametrization not have any arbitrary boundary condition B_c, but because our new definite resonance energies $\mathcal{E}_\lambda$ are poles of the scattering matrix, these physical quantities are also independent of the channel radius a_c (though the other introduced parameters, the Ducru definite resonance widths $\alpha_{\lambda,c}$, are not). Moreover, the real and imaginary parts of these definite levels $\mathcal{E}_\lambda$ are thus the natural variables with which to describe the physical resonances. The main drawback of our parametrization is that all the parameters are now complex numbers (somewhat complicating the documentation), constrained to a hypersurface with no known explicit description to date, thereby compromising the direct evaluation of these parameters. Just as we did for the Brune parametrization in [14], we also establish the existence of shadow poles in this definite parametrization of R-matrix theory, and show that these can be ignored and still exactly parametrize nuclear cross sections. We concomitantly show that, somewhat peculiarly, one can also fully reconstruct nuclear cross sections using the shadow poles instead of the principal poles.

Evidence of all these properties is observed in xenon isotope ^{134}Xe spin-parity group $J^\pi = 1/2^{(-)}$, and is presented in Sec. IV.

II. WIGNER-EISENBUD AND REICH-MOORE PARAMETRIZATIONS OF *R*-MATRIX CROSS SECTIONS

We here summarize the Wigner-Eisenbud parametrization of R-matrix theory, as well as its Reich-Moore extension, which underpin modern nuclear data libraries.

A. Scattering theory and cross sections

General scattering theory expresses the incoming channel c and outgoing channel c' angle-integrated partial cross section $\sigma_{c,c'}(E)$ at energy E as a function of the probability *transition matrix* $T_{cc'}(E)$, according to Eq. (3.2d), Sec. VIII 3. p. 293 of [2]:

$$\sigma_{cc'}(E) \;=\; 4\pi\, g_{J_c^\pi} \left| \frac{T_{cc'}(E)}{k_c(E)} \right|^2, \tag{1}$$

where k_c is the wave number of the channel, and $g_{J_c^\pi}$ the *spin statistical factor* defined as (Eq. (3.2c), Sec. VIII 3, p. 293 of [2])

$$g_{J_c^\pi} \;\triangleq\; \frac{2J_c+1}{(2I_1+1)(2I_2+1)}, \tag{2}$$

where J_c^π is the total angular momentum of the channel (with its parity π), and I_1, I_2 the spins of the two interacting bodies. The transition matrix is itself derived from the *scattering matrix* $\boldsymbol{U}$ of the interaction (cf. Eq (7) of [27]),

$$\boldsymbol{T} \;\triangleq\; \frac{\mathbb{I} - \boldsymbol{e}^{-i\boldsymbol{\omega}}\boldsymbol{U}\boldsymbol{e}^{-i\boldsymbol{\omega}}}{2} \tag{3}$$

where $\boldsymbol{\omega} \triangleq \mathbf{diag}(\omega_c)$ is the diagonal matrix composed of $\omega_c \triangleq \sigma_{\ell_c}(\eta_c) - \sigma_0(\eta_c)$, that is the differences in *Coulomb phase shift*, $\sigma_{\ell_c}(\eta_c)$, which are linked to the phases (argument) of the gamma function as defined by Thompson in Eq. (33.2.10) of [29] for angular momentum ℓ_c:

$$\sigma_{\ell_c}(\eta_c) \;\triangleq\; \arg(\Gamma(1+\ell_c+i\eta_c)) \tag{4}$$

and the *dimensionless Coulomb field parameter*,

$$\eta_c \;\triangleq\; \frac{Z_1 Z_2 e^2 M_\alpha r_c}{\hbar^2 \rho_c}, \tag{5}$$

where r_c is the radial distance coordinate of channel c, e the elementary charge, $\hbar$ the Planck constant, Z_1 and Z_2 the charge

numbers in the two interacting bodies, M_α the reduced mass of the system, and ρ_c the dimensionless wave number,

$$\rho_c \triangleq k_c\, r_c, \tag{6}$$

product of the wave number k_c and the channel radial coordinate r_c. Note that transition matrix (3) definition $T_{cc'} \triangleq \frac{\delta_{cc'} - e^{-i\omega_c} U_{cc'} e^{-i\omega_{c'}}}{2}$ is a scaled rotation of the one defined by Lane and Thomas, $T^{\text{L\&T}}_{cc'} \triangleq \delta_{cc'} e^{2i\omega_c} - U_{cc'}$ (cf. Eq. (2.3), Sec. VIII 2, p. 292 and Eq.(3.2d), Sec. VIII 3, p. 293 of [2]), that we introduce for better physical interpretability, algebraic simplicity, and numerical stability.

Unitarity of the scattering matrix entails that the total cross section of a given channel is then

$$\sigma_c(E) \triangleq \sum_{c'} \sigma_{cc'}(E) = 4\pi\, g_{J^\pi_c} \frac{\text{Re}\,[T_{cc}(E)]}{|k_c(E)|^2}. \tag{7}$$

B. Scattering matrix Wigner-Eisenbud and Reich-Moore *R*-matrix parametrizations

R-matrix theory, as best described by Bloch in [1] (see Kapur and Peierls [3], and Wigner and Eisenbud [4] seminal works, as well as the Lane and Thomas review [2]), is a way of parametrizing the energy dependence of the scattering matrix $\boldsymbol{U}(E)$ in order to easily compute the cross sections using expressions (1), (3), and (7).

For each channel, an arbitrary *channel radius* a_c is set to separate the space into two regions: an outer region ($r_c > a_c$) where the Hamiltonian of the system is well known (say Coulomb repulsion or free particle), and an inner region ($r_c < a_c$) where the forces interacting are considered an intractable "black box." Using Green's theorem and projecting upon the $r_c = a_c$ surface allows one to formally solve for and parametrize the scattering matrix (cf. Bloch's Eqs. (31), (34), (43), and (50) in [1]). We therefore perform such projection, and shall henceforth have $r_c = a_c$ in all subsequent expressions.

For calculability reasons, Wigner and Eisenbud completely parametrized the scattering matrix by introducing an arbitrary, real, fixed boundary condition B_c for each channel (cf. Eqs. (55) and (60) of [1]), whereupon the Wigner-Eisenbud *resonance parameters* consist of a set of boundary conditions B_c, *resonance energies* E_λ, and *resonance widths* $\gamma_{\lambda,c}$ (also known as *reduced width amplitudes*), which are documented in standard nuclear data libraries (ENDF [5], JEFF [6], BROND [7], JENDL [8], CENDL [9], TENDL [10,11]), and are a keystone of our knowledge of nuclear physics.

R-matrix theory then parametrizes the scattering matrix with these resonance parameters as follows:

$$\boldsymbol{U} = \boldsymbol{O}^{-1}\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}\boldsymbol{\gamma}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{\gamma}\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}, \tag{8}$$

where the *level matrix* $\boldsymbol{A}$ (cf. Eqs. (17) and (18) of Sec. II C of [14]) is defined as

$$\boldsymbol{A^{-1}} \triangleq \boldsymbol{e} - E\mathbb{I} - \boldsymbol{\gamma}(\boldsymbol{L} - \boldsymbol{B})\boldsymbol{\gamma}^{\mathsf{T}}, \tag{9}$$

where $\boldsymbol{B} = \mathbf{diag}(B_c)$ is the diagonal matrix of real arbitrary boundary conditions B_c, and where we built the diagonal matrix of resonance energies $\boldsymbol{e} \triangleq \mathbf{diag}(E_\lambda)$ [of size N_λ, the number of levels (resonances)] and the rectangular matrix of resonance widths $\boldsymbol{\gamma} = \mathbf{mat}(\gamma_{\lambda,c})$ (of size $N_\lambda \times N_c$, where N_c is the number of channels). Except for these parameter matrices $\boldsymbol{e}$, $\boldsymbol{\gamma}$, and $\boldsymbol{B}$, all other matrices in (8) and (9) are functions of energy E (cf. Sec. II D).

In exact *R*-matrix theory, these resonance parameters $\{E_\lambda, \gamma_{\lambda,c}\}$ are real, but they can become complex in the Reich-Moore formalism. Indeed, the *Reich-Moore approximation* [16] focuses on a subset of all possible outcomes (channels c) of a given nuclear reaction (such as neutron fission, scattering, photon emissions, etc.), which it describes explicitly, and "eliminates" all other channels (usually "gamma capture" photon channels denoted γ)—cf. the Teichmann and Wigner [30] channel elimination method, Chap. X in [2]—modeling their effects on the explicitly treated channels by adding to every level's resonance energy E_λ a shift into the complex plane called *eliminated capture width* $\Gamma_{\lambda,\gamma}$:

$$\boldsymbol{e}_{\text{R.M.}} \triangleq \mathbf{diag}_\lambda\left(E_\lambda - i\frac{\Gamma_{\lambda,\gamma}}{2}\right). \tag{10}$$

From this, the Reich-Moore formalism inverse level matrix (9), where all the eliminated capture channels have been collapsed into one γ channel, is now defined as

$$\boldsymbol{A^{-1}}_{\text{R.M.}} \triangleq \boldsymbol{e}_{\text{R.M.}} - E\,\mathbb{I} - \boldsymbol{\gamma}(\boldsymbol{L} - \boldsymbol{B})\boldsymbol{\gamma}^{\mathsf{T}} \tag{11}$$

Since the other *R*-matrix expressions linking these operators to the scattering matrix (8), and thereby the cross section (1), remain unchanged, the only practical effect of the Reich-Moore formalism is that it allows for complex resonance energies (10). In this sense, we can see the Reich-Moore formalism as a generalization of the exact *R*-matrix formalism, even though it initially came from an approximation to eliminate intractable channels. However, because this Reich-Moore approximation breaks the unitarity of the scattering matrix, summing the partial cross sections (1) over the noneliminated channels no longer adds-up to the total cross section (7)—now defined as the right-hand expression of (7)—and the difference defines the *eliminated* γ*-capture cross section*.

The Reich-Moore formalism is of particular importance for heavy nuclides (which are large many-body problems), where we are often unable to track the vast number of all possible channels (say every single individual photon interaction).

Henceforth, we shall thus treat *R*-matrix theory in this generalized framework, where the scattering matrix (8) is expressed as a function of the level matrix (9), with real channel widths $\gamma_{\lambda,c}$, but complex resonance energies as in (10).

C. Outer region *R*-matrix wave functions

The last operators remaining to fully describe the scattering matrix in (8) and (9) are the dimensionless reduced logarithmic derivatives of the outgoing wave function at the channel surface, $\boldsymbol{L} = \mathbf{diag}(L_c)$, where $L_c(\rho_c)$ are defined as

$$L_c(\rho_c) \triangleq \frac{\rho_c}{O_c}\frac{\partial O_c}{\partial \rho_c}, \tag{12}$$

and the incoming and outgoing waves, $\boldsymbol{I} = \mathbf{diag}(I_c)$ and $\boldsymbol{O} = \mathbf{diag}(O_c)$—functions of the dimensionless wave number $\rho_c \triangleq a_c k_c$ and subject to the Wronksian condition for all channels

c, $w_c \triangleq O_c^{(1)} I_c - I_c^{(1)} O_c = 2\mathrm{i}$—which are linked to the regular and irregular Coulomb wave functions (or Bessel functions in the case of neutral particle channels), defined in Eqs. (2.13a)–(2.13b), Sec. III 2 b, p. 269 of [2]:

$$\begin{aligned} O_c &= H_{+c} e^{-i\omega_c} = (G_c + iF_c) e^{-i\omega_c}, \\ I_c &= H_{-c} e^{i\omega_c} = (G_c - iF_c) e^{i\omega_c}, \end{aligned} \tag{13}$$

and for properties of which we refer to Ian J. Thompson's Chap. 33, Eq. (33.2.11) in [29], or Abramowitz and Stegun, Chap. 14, p. 537 [31]. In [14], we established the Mittag-Leffler expansions of both O_c and L_c (cf. Theorem 1, Eqs. (13) and (16) of [14]), which may be another way of effectively computing these operators.

D. Energy–wave-number mapping

The total energy of the system, E, is the eigenvalue of the Hamiltonian in the reduced center-of-mass frame. Each channel c has its own kinetic energy E_c, and energy conservation can be expressed by means of the relativistic and channel invariant Mandelstam variable s, which is the square of the relativistic center-of-mass energy of the two bodies composing any channel c, with respective masses $m_{c,1}$ and $m_{c,2}$ (null for photons),

$$\begin{aligned} s &= (E_c + (m_{c,1} + m_{c,2})\, c^2)^2 \\ &= (E_{c'} + (m_{c',1} + m_{c',2})\, c^2)^2 = \cdots, \quad \forall\, c. \end{aligned} \tag{14}$$

Each channel also has its wave number k_c, which is related to the energy E according to an energy–wave-number mapping,

$$k_c(E) \quad \longleftrightarrow \quad E, \tag{15}$$

which can be generally described for all channels using the special relativity expression

$$k_c = \sqrt{\frac{[s - (m_{c,1} + m_{c,2})^2 c^4][s - (m_{c,1} - m_{c,2})^2 c^4]}{4\hbar^2 c^2\, s}}. \tag{16}$$

In the semiclassical limit of (16), energy conservation cannot be respected below a certain threshold energy E_{T_c} [cf. Eq. (5.12), p. 557 of [17]), where $E_{T_c} = 0$ for reactions without threshold. A channel composed of two massive particles (i.e., not photons), of respective masses $m_{c,1}$ and $m_{c,2}$ will then have a wave number k_c tending to

$$k_c(E) = \sqrt{\frac{2 m_{c,1} m_{c,2}}{(m_{c,1} + m_{c,2})\hbar^2}(E - E_{T_c})}. \tag{17}$$

In the same semiclassical limit, for a photon particle interacting with a massive body of mass $m_{c,1}$, the center-of-mass wave number k_c is linked to the total center-of-mass energy E according to

$$k_c(E) = \frac{(E - E_{T_c})}{2\hbar c}\left[1 + \frac{m_{c,1} c^2}{(E - E_{T_c}) + m_{c,1} c^2}\right]. \tag{18}$$

Regardless of the approach taken, all these energy–wave-number mappings (15) require choosing the sign of the square root $\pm\sqrt{\cdot}$ in (16), whence these $k_c(E)$ relations engender a complex multisheeted Riemann surface with branch points at (or close to) the threshold energies E_{T_c}, as discussed in Sec. II A, p. 2 of [14].

The outgoing O_c and incoming I_c wave functions, and thus also L_c, are defined as variables of ρ_c, and careful consideration must therefore be applied in specifying the $\pm$ branch chosen when mapping E to $k_c(E)$, as discussed in detail in both [14] and [28].

III. DEFINITE PARAMETRIZATION OF *R*-MATRIX THEORY

We here establish our definite parametrization of R-matrix theory, showing it is complete and invariant, and further discuss some of its salient properties.

A. Defining the definite parametrization of *R*-matrix theory

In the Wigner-Eisenbud parametrization, the scattering matrix $\boldsymbol{U}$ is expressed with the level matrix $\boldsymbol{A}$ according to (8). Similarly, in our definite parametrization of R-matrix theory, the scattering matrix is expressed with the *Ducru definite level matrix* $\boldsymbol{D}$ as

$$\boldsymbol{U} = \boldsymbol{O}^{-1}\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}\boldsymbol{\alpha}^{\mathsf{T}}\boldsymbol{D}\boldsymbol{\alpha}\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}, \tag{19}$$

where $[\,\cdot\,]^{\mathsf{T}}$ designates the transpose (not the Hermitian conjugate), and $\boldsymbol{\alpha} \triangleq \mathbf{mat}(\alpha_{\lambda,c})$ is the matrix of *Ducru definite resonance widths*, which, together with the *Sigert-Humblet radioactive state energies* (or *definite levels*) $\mathcal{E}_\lambda$, are complex numbers constituting the new *definite resonance parameters*. These definite resonance parameters themselves parametrize the definite level matrix $\boldsymbol{D}$ through its *Moore-Penrose pseudo inverse* [32,33] (denoted $[\,\cdot\,]^{+}$) as

$$\boldsymbol{D}^{+} = \boldsymbol{Q} - E(\mathbb{I} + \boldsymbol{W}) - \boldsymbol{\alpha}\boldsymbol{L}(E)\boldsymbol{\alpha}^{\mathsf{T}} \tag{20}$$

with $\mathbb{I}$ designating the identity matrix,

$$W_{\lambda\mu} \triangleq \begin{cases} \sum_{c=1}^{N_c} \alpha_{\lambda,c}\left(\frac{L_c(\mathcal{E}_\mu) - L_c(\mathcal{E}_\lambda)}{\mathcal{E}_\lambda - \mathcal{E}_\mu}\right)\alpha_{\mu,c}, & \forall\, \lambda \neq \mu, \\ 0, & \forall\, \lambda = \mu, \end{cases} \tag{21}$$

and

$$Q_{\lambda\mu} \triangleq \begin{cases} \sum_{c=1}^{N_c} \alpha_{\lambda,c}\left(\frac{L_c(\mathcal{E}_\mu)\mathcal{E}_\lambda - L_c(\mathcal{E}_\lambda)\mathcal{E}_\mu}{\mathcal{E}_\lambda - \mathcal{E}_\mu}\right)\alpha_{\mu,c}, & \forall\, \lambda \neq \mu, \\ \mathcal{E}_\lambda + \sum_{c=1}^{N_c} \alpha_{\lambda,c} L_c(\mathcal{E}_\lambda)\alpha_{\lambda,c}, & \forall\, \lambda = \mu. \end{cases} \tag{22}$$

Note that the $Q_{\lambda\mu}$ matrix elements can equivalently be expressed as

$$\begin{aligned} Q_{\lambda\mu} &= \frac{\mathcal{E}_\lambda + \mathcal{E}_\mu}{2}(\delta_{\lambda,\mu} + W_{\lambda\mu}) \\ &\quad + \sum_{c=1}^{N_c} \alpha_{\lambda,c}\left(\frac{L_c(\mathcal{E}_\lambda) + L_c(\mathcal{E}_\mu)}{2}\right)\alpha_{\mu,c}. \end{aligned} \tag{23}$$

Thought complex, the definite parameters are therefore analogous to the traditional Wigner-Eisenbud R-matrix parameters in that to each real level E_λ there corresponds a complex definite level $\mathcal{E}_\lambda$, and to each real resonance width $\gamma_{\lambda,c}$ there corresponds a complex definite resonance

width $\alpha_{\lambda,c}$. From this perspective, our definite parametrization (19)—constituted of the (20) definite level matrix $\boldsymbol{D}$, the definite levels $\mathcal{E}_\lambda$ (which are poles of the scattering matrix $\boldsymbol{U}$), and the definite resonance widths $\alpha_{\lambda,c}$—is complete (see Sec. III C), and equivalent to the traditional Wigner-Eisenbud parametrization (8). As we will show in Sec. III D, the definite level matrix (20) is invariant to boundary parameters B_c, but not to channel radii a_c (and thus nor are the widths $\alpha_{\lambda,c}$), though its poles $\mathcal{E}_\lambda$ are.

B. Constructing the definite parameters from the Wigner-Eisenbud *R* matrix

In order to guarantee this equivalence with the traditional Wigner-Eisenbud parametrization (8), we construct the definite resonance widths $\alpha_{\lambda,c}$ and the definite level matrix $\boldsymbol{D}$ such that the following equality stands:

$$\boldsymbol{\alpha}^\mathsf{T}\boldsymbol{D}\boldsymbol{\alpha} \;=\; \boldsymbol{\gamma}^\mathsf{T}A\boldsymbol{\gamma} \tag{24}$$

whence the scattering matrix $\boldsymbol{U}$ is left unchanged in (19). For this, we define the Ducru definite level matrix $\boldsymbol{D}$ from the Wigner-Eisenbud level matrix $\boldsymbol{A}$ as the pseudoinverse:

$$\boldsymbol{D}(E) \;\triangleq\; [\boldsymbol{V}^\mathsf{T}\boldsymbol{A}^{-1}(E)\boldsymbol{V}]^{+}, \tag{25}$$

where the $\boldsymbol{V}$ matrix is composed of the size-N_c column eigenvectors, $\boldsymbol{V} \triangleq [\boldsymbol{v_1}, \ldots, \boldsymbol{v_\lambda}, \ldots, \boldsymbol{v}_{N_L}]$, which are the solutions to the following *definite (or radioactive) states* generalized eigenproblem:

$$[\boldsymbol{e}_{\text{R.M.}} - \boldsymbol{\gamma}(\boldsymbol{L}(\mathcal{E}_\lambda) - \boldsymbol{B})\boldsymbol{\gamma}^\mathsf{T}]\boldsymbol{v_\lambda} = \mathcal{E}_\lambda \boldsymbol{v_\lambda}, \tag{26}$$

where we assume we can pseudonormalize the eigenvectors as

$$\boldsymbol{v}_\lambda^\mathsf{T}\boldsymbol{v_\lambda} = 1. \tag{27}$$

Note that because the vectors are now complex, the latter is not a norm and this pseudonormalization is not always possible (for instance $[i, 1] \cdot [i, 1]^\mathsf{T} = 0$). In practice, however, the probability of this happening is almost always null (see Sec. IV C of [28] for further discussion).

We then define the definite parameters as

(i) the definite levels $\mathcal{E}_\lambda$: these are the Siegert-Humblet radioactive state resonance energies, which are complex and we proved to exactly be the poles of the scattering matrix $\boldsymbol{U}(E)$ (cf. theorem 3 in [28]);

(ii) the Ducru definite resonance widths $\alpha_{\lambda,c}$ (which are also complex), which we define as

$$\boldsymbol{\alpha} \triangleq \boldsymbol{V}^\mathsf{T}\boldsymbol{\gamma}. \tag{28}$$

Injecting definition (28), radioactive states relation (26), and the pseudonormalization condition (27) into the definite level matrix definition (25) yields explicit expressions (20), (21), (22), and (23).

Given a set of Wigner-Eisenbud resonance parameters $\{E_\lambda, \gamma_{\lambda,c}\}$, the key to constructing the definite parameters $\{\mathcal{E}_\lambda, \alpha_{\lambda,c}\}$ is therefore solving the definite states eigenproblem (26), and we will see in Sec. III C we only need N_λ out of its total number N_L of solutions. The definite states eigenproblem (26) is a type of generalized nonlinear eigenproblem, composed of complex symmetric matrices. Numerical algorithms to solve this type of problem can be found in *The Handbook of Linear Algebra* (Chap. 115 of [34]), and can be enhanced with complex-symmetric features such as the Lanczos method [35]. To solve the definite states eigenproblem (26), some authors have also sometimes found it more convenient to first solve the corresponding determinant null-space problem (see [36], Eqs. (200) and (204) of [37], or the last paragraphs of Sec. V of [12]):

$$\det(\boldsymbol{e}_{\text{R.M.}} - E\,\mathbb{I} - \boldsymbol{\gamma}[\boldsymbol{L}(E) - \boldsymbol{B}]\boldsymbol{\gamma}^\mathsf{T})|_{E=\mathcal{E}_\lambda} = 0, \tag{29}$$

which can be simpler to solve when the number of levels is much smaller than the number of channels ($N_\lambda \ll N_c$). Conversely, if there are many more channels than levels ($N_c \gg N_\lambda$), it can be simpler to find the definite levels $\mathcal{E}_\lambda$ by solving

$$\det(\mathbb{I} - \boldsymbol{R}_{\text{R.M.}}(E)[\boldsymbol{L}(E) - \boldsymbol{B}])|_{E=\mathcal{E}_\lambda} = 0, \tag{30}$$

where $\boldsymbol{R}_{\text{R.M.}}(E) \triangleq \boldsymbol{\gamma}^\mathsf{T}(\boldsymbol{e}_{\text{R.M.}} - E\,\mathbb{I})^{-1}\boldsymbol{\gamma}$ is the Wigner-Eisenbud R matrix, with Reich-Moore complex resonance energies (10). Determinant problem (30) yields equivalent $\mathcal{E}_\lambda$ results to (29) due to Woodbury identity (see Eq. (21) in [14]). We refer the reader to Sec. II C. of [28] for more ample discussion as to how to solve the definite levels state eigenproblem (26).

C. Completeness and choice of parameters

By construction, the definite parameters $\{\mathcal{E}_\lambda, \alpha_{\lambda,c}\}$ are complete in the sense that they suffice to fully reconstruct the scattering matrix (19), and therefore the cross sections (1) and (7). This is because the properties of the Moore-Penrose pseudoinverse guarantee (24) will be satisfied through definitions (25) and (28), as long as $\boldsymbol{V}$ has more linearly independent columns than rows [32,33], which is always satisfied in practice with $N_L \geqslant N_\lambda$.

This has important consequences. Indeed, we showed in Theorem 1 of [28] there are more than N_λ definite levels $\mathcal{E}_\lambda$ (poles of the scattering matrix $\boldsymbol{U}$) that will solve the radioactive states generalized eigenproblem (26), necessary to construct the definite resonance widths (28). In fact, on every sheet of the energy–wave-number mapping (15), each resonance energy E_λ generates two solutions to (26) (one on each $\pm\sqrt{\cdot}$ branch), and each pole ω_n of the outgoing wave function reduced logarithmic derivative operator $L_c(\rho_c)$ (documented in Tables I and II of [14]) adds another solution to (26), so that the total number N_L of solutions to (26) is a (countable) infinity $N_L = \infty$ for charged particles, and

$$N_L = \left(2N_\lambda + \sum_{c=1}^{N_c} \ell_c\right) \times 2^{(N_{E_{T_c} \neq E_{T_{c'}}} - 1)} \tag{31}$$

for neutral particles, where $N_{E_{T_c} \neq E_{T_{c'}}}$ is the number of channels with different thresholds (cf. Eq. (34) of [28]). As explained in Theorem 1 of [28], this entails that one must specify on which $\pm$ sheet of the energy–wave-number mapping (15) each of the definite levels $\mathcal{E}_\lambda$ resides. For each energy—invariant Mandelstam variable s in (14)—there are two wave numbers k_c based on the choice of $\pm\sqrt{\cdot}$ sign in the branches of mapping (15): one in the physical sheet (as defined as $\text{Im}[k_c] > 0$) and one in the unphysical sheet (for $\text{Im}[k_c] < 0$). The scattering

TABLE I. Definite parameters—definite levels $\mathcal{E}_\lambda$ (Siegert-Humblet radioactive state resonance energies, poles of the scattering matrix) and Ducru definite resonance widths $\alpha_{\lambda,c}$ of the definite parametrization (20) of R-matrix theory (19)—of the two p-wave resonances of ^{134}Xe, spin-parity group $J^\pi = 1/2^{(-)}$, converted from the Wigner-Eisenbud R-matrix parameters reported in ENDF/B-VIII.0 (MLBW evaluation) using the Reich-Moore level matrix (11) in R-matrix parametrization (8).

$z = \sqrt{E}$ (with E in eV)
$A = 132.7600$
$a_c = 5.80$: channel radius (fermis)
$\rho_0 = \frac{Aa_c\sqrt{\frac{2m_n}{\hbar}}}{A+1}$ $(\sqrt{\text{eV}}^{-1})$, so that $\rho(z) \triangleq \rho_0 z$
with $\sqrt{\frac{2m_n}{\hbar}} = 0.002\,196\,807\,122\,623$ $[1/(10^{-14}\ \text{m}\sqrt{\text{eV}})]$

Definite parameters (rounded to 5 digits)

Definite levels $\{\mathcal{E}_\lambda, \pm\}$ from (26) (eV), sheet of (15)	Definite resonance widths $\alpha_{\lambda,c}$ from (28) $(\sqrt{\text{eV}})$
$\{-6.2694 \times 10^{+5} - i1.0238 \times 10^{-4}, +\}$	$2.8122 \times 10^{+1} + i2.7436 \times 10^{-9}$
$\{2.1838 \times 10^{+3} + i9.0757 \times 10^{-2}, -\}$	$2.5126 \times 10^{+1} - i2.4846 \times 10^{-4}$
$\{2.1838 \times 10^{+3} - i1.6868 \times 10^{-1}, +\}$	$2.5126 \times 10^{+1} + i2.4831 \times 10^{-4}$
$\{6.3130 \times 10^{+3} + i1.6025 \times 10^{-1}, -\}$	$1.4087 \times 10^{+1} + i2.1627 \times 10^{-3}$
$\{6.3130 \times 10^{+3} - i2.3822 \times 10^{-1}, +\}$	$1.4087 \times 10^{+1} - i2.1625 \times 10^{-3}$

Wigner-Eisenbud R-matrix parameters

$E_1 = 2186.0$: first resonance energy (eV)
$\Gamma_{1,n} = 0.2600$: neutron width of first resonance (not reduced width), i.e., $\Gamma_{\lambda,c} = 2P_c(E_\lambda)\gamma^2_{\lambda,c}$
$\Gamma_{1,\gamma} = 0.0780$: eliminated capture width (eV)
$E_2 = 6315.0$: second resonance energy (eV)
$\Gamma_{2,n} = 0.4000$ (eV)
$\Gamma_{2,\gamma} = 0.0780$ (eV)
$g_{J^\pi} = 1/3$: spin statistical factor
$B_c = -1$

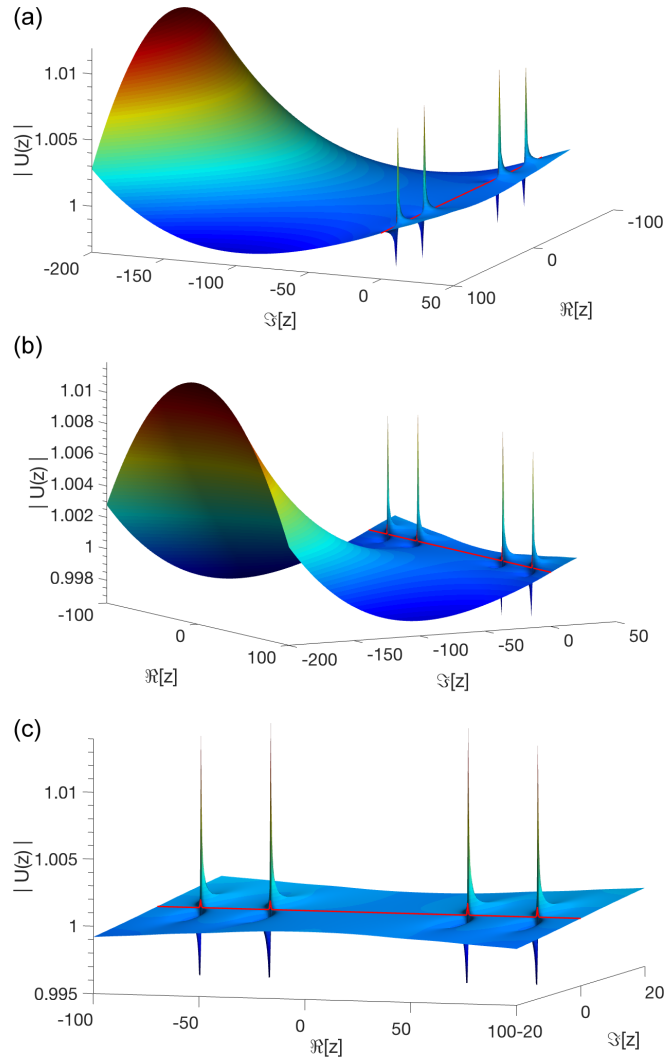

FIG. 1. Scattering matrix of ^{134}Xe two p-wave resonances in spin-parity group $J^\pi = 1/2^{(-)}$. (a) Scattering matrix modulus surface. (b) Two principal resonant poles, two shadow poles, and one outer pole. (c) Principal and shadow poles along the real z axis. Dimensionless $|\boldsymbol{U}|(z)$ is computed using nuclear data parameters from Table I, using either the Wigner-Eisenbud parametrization (8) with Reich-Moore level matrix (11), or the definite parametrization (19), yielding identical complex values. The surface presents two principal resonant poles near the resonances on the positive z axis, where $z^2 = E$, and each of these presents a shadow pole on the negative z axis. A fifth, very large, principal outer "angular momenta scattering pole" is present along the imaginary z axis, far off the real z axis. The modulus of the scattering matrix along the real z axis is here depicted as a red line on the surface.

matrix poles $\mathcal{E}_\lambda$ on the negative sheet of mapping (15) are named "shadow poles" [38], whereas the poles on the positive sheet are called "principal poles."

A remarkable result deriving from our definition (28), guaranteed by construction through (25), is that one can choose any subset of the N_L solutions to (26) to fully and exactly reconstruct the scattering matrix $\boldsymbol{U}(E)$, as long as we choose at least N_λ of them.

This means we can always choose only N_λ solutions to (26), and construct the corresponding definite parameters. This choice is not *a priori* unique, though it can be prescribed as such through convention, for instance by always choosing the scattering matrix pole $\mathcal{E}_\lambda$ which is closest to the real resonance energy E_λ on the $+\sqrt{\cdot}$ sheet of the energy–wavenumber mapping (15). But one can also choose more solutions $N_L \geqslant N_\lambda$ to reproduce the same results, or only choose N_λ solutions that correspond to shadow poles and not principal poles. Evidence of this somewhat surprising phenomenon is observed in the spin-parity group $J^\pi = 1/2^{(-)}$ of xenon isotope ^{134}Xe and documented in Sec. IV, where one can pick any two of the five possible definite parameters in Table I to exactly compute the scattering matrix using (19), complete with its five poles as shown in Fig. 1.

This result is due to the fact that the pseudoinverse in expression (20) will collapse the linearly dependent solutions

of (26) to yield the same scattering matrix. In this sense, our definite parametrization is complete, but not unique (though it can be made unique by convention).

D. Invariance of parameters

We proved in Theorem 3 of [28] that the Siegert-Humblet radioactive states resonance energies $\mathcal{E}_\lambda$ (definite levels) are exactly the poles of the scattering matrix $\boldsymbol{U}(E)$, and, as such, they are invariant with respect to both the arbitrary boundary conditions B_c and channel radii a_c (cf. Eq. (47), Theorem 2 in [28]):

$$\frac{\partial \mathcal{E}_\lambda}{\partial B_c} = 0, \quad \frac{\partial \mathcal{E}_\lambda}{\partial a_c} = 0. \tag{32}$$

In this sense, our definite parametrization of R-matrix theory is composed of invariant (complex) resonance energies $\mathcal{E}_\lambda$ with strong physical properties.

To keep the scattering matrix unchanged by a change of boundary condition from $\boldsymbol{B}$ to $\boldsymbol{B}'$, the resonance energies $\boldsymbol{e}$ and resonance levels $\boldsymbol{\gamma}$ must be changed in such a way that $\boldsymbol{R}_{\boldsymbol{B}}^{-1} + \boldsymbol{B} = \boldsymbol{R}_{\boldsymbol{B}'}^{-1} + \boldsymbol{B}'$, where $\boldsymbol{R}(E) \triangleq \boldsymbol{\gamma}^\mathsf{T}(\boldsymbol{e} - E\mathbb{I})^{-1}\boldsymbol{\gamma}$ is Wigner's R matrix (cf. Eq. (4) of [13]). Using the Woodbury identity twice, this translates into the following relation linking the R matrices of two different boundary conditions:

$$\boldsymbol{R}_{\boldsymbol{B}'} = \boldsymbol{\gamma}_{\boldsymbol{B}}^\mathsf{T}\big[\boldsymbol{e}_{\boldsymbol{B}} - E\mathbb{I} + \boldsymbol{\gamma}_{\boldsymbol{B}}(\boldsymbol{B} - \boldsymbol{B}')\boldsymbol{\gamma}_{\boldsymbol{B}}^\mathsf{T}\big]^{-1}\boldsymbol{\gamma}_{\boldsymbol{B}}. \tag{33}$$

Barker showed in [13] that this leads to a resonance parameters transformation under change of boundary condition $\boldsymbol{B} \to \boldsymbol{B}'$ which can be performed by diagonalizing,

$$\boldsymbol{C} \triangleq \boldsymbol{e}_{\boldsymbol{B}} + \boldsymbol{\gamma}_{\boldsymbol{B}}(\boldsymbol{B} - \boldsymbol{B}')\boldsymbol{\gamma}_{\boldsymbol{B}}^\mathsf{T} = \boldsymbol{K}^\mathsf{T}\boldsymbol{e}_{\boldsymbol{B}'}\boldsymbol{K}, \tag{34}$$

where $\boldsymbol{K}^\mathsf{T}\boldsymbol{K} = \mathbb{I}$, and defining the transformed Wigner-Eisenbud resonance widths under boundary condition change $\boldsymbol{B} \to \boldsymbol{B}'$ as

$$\boldsymbol{\gamma}_{\boldsymbol{B}'} \triangleq \boldsymbol{K}\boldsymbol{\gamma}_{\boldsymbol{B}}. \tag{35}$$

In the original Wigner-Eisenbud R-matrix formalism, all the resonance parameters and the boundary condition are real, so that $\boldsymbol{C}$ is a real symmetric matrix whose orthogonal diagonalization (34) is therefore guaranteed by the spectral theorem. However, when we seek to generalize this transformation (35) to the Reich-Moore formalism, the fact the the resonance energies (10) are now complex (shifted into the complex plane by the eliminated capture widths) entails that $\boldsymbol{C}$ is a complex symmetric matrix (not Hermitian), and its diagonalization (34) is therefore no longer guaranteed, but must instead be assumed. Since diagonalizable matrices are dense in the space of complex matrices, this assumption is unlikely to be a limiting factor in practice, but it is nonetheless an assumption. To generalize the transformation to the Reich-Moore formalism, we thus assume that complex symmetric $\boldsymbol{C}$ is diagonalizable (34) but no longer by real matrices nor with a real spectrum, from which it follows that $\boldsymbol{K}$ must satisfy $\boldsymbol{K}^{-1} = \boldsymbol{K}^\mathsf{T}$.

To establish the invariance of the definite resonance widths $\alpha_{\lambda,c}$ with respect to a change of boundary conditions $\boldsymbol{B} \to \boldsymbol{B}'$, it then suffices to consider the left-hand side of the radioactive states generalized eigenproblem (26), define the matrix $\boldsymbol{\Lambda}_{\boldsymbol{B}}(E) \triangleq \boldsymbol{e}_{\boldsymbol{B}} - \boldsymbol{\gamma}_{\boldsymbol{B}}[\boldsymbol{L}(E) - \boldsymbol{B}]\boldsymbol{\gamma}_{\boldsymbol{B}}^\mathsf{T}$ which is being diagonalized, and note that under a change of boundary conditions $\boldsymbol{B} \to \boldsymbol{B}'$ it satisfies $\boldsymbol{\Lambda}_{\boldsymbol{B}'}(E) = \boldsymbol{K}\boldsymbol{\Lambda}_{\boldsymbol{B}}(E)\boldsymbol{K}^\mathsf{T}$. Whence, the radioactive eigenvectors satisfy $\boldsymbol{v}_\lambda^{\boldsymbol{B}'} = \boldsymbol{K}\boldsymbol{v}_\lambda^{\boldsymbol{B}}$, which guarantees the invariance of definite resonance widths to a change of boundary parameters, according to $\boldsymbol{\alpha}_\lambda^{\boldsymbol{B}'} = \boldsymbol{v}_\lambda^{\boldsymbol{B}'\mathsf{T}}\boldsymbol{\gamma}_{\boldsymbol{B}'} = \boldsymbol{v}_\lambda^{\boldsymbol{B}\mathsf{T}}\boldsymbol{K}^\mathsf{T}\boldsymbol{\gamma}_{\boldsymbol{B}'} = \boldsymbol{v}_\lambda^{\boldsymbol{B}\mathsf{T}}\boldsymbol{\gamma}_{\boldsymbol{B}} = \boldsymbol{\alpha}_\lambda^{\boldsymbol{B}}$.

Therewith, the definite resonance widths $\alpha_{\lambda,c}$ are invariant to a change of boundary conditions (like Brune's in the case of R-matrix formalism without Reich-Moore eliminated capture widths; see Sec. III H for further discussion), and furthermore the definite levels $\mathcal{E}_\lambda$ are also invariant with respect to changes in channel radii (Brune's alternative resonance energies are not).

E. Definite parameters implicit constraints

What about the definite resonance widths $\alpha_{\lambda,c}$ transformation under change of channel radii a_c? We were unable to derive an explicit formulation for such transformation, though an implicit one is possible.

Indeed, in Theorem 2 of [28], we established the differential equation (48) to which the widths of the residues $\boldsymbol{r}_\lambda$ of the *Kapur-Peierls operator*, $\boldsymbol{\gamma}^\mathsf{T}\boldsymbol{A}\boldsymbol{\gamma}$, are subject (assuming semisimplicity and nondegenerate states; see Eq. (57) of [28] for degenerate states, and Sec. IV C of [28] for further discussion). We can here take a similar approach, and adapt the Gohberg-Sigal theory to complex-symmetric matrices by assuming—on physical quasi-null likelihood of occurrence arguments—nondefective eigenvectors, semisimplicity, and nondegenerate poles (see article [28], Sec. II A, Eq. (10) and the discussion immediately preceding Eq. (13), as well as Secs. IV C and IV D, Lemma 1, Eqs. (62) and (64) for further discussion), so as to write the definite level matrix Mittag-Leffler expansion with simple poles of Laurent order 1 and rank-1 residues in a neighborhood $\mathcal{W}(E)$ of the definite levels:

$$\boldsymbol{D}(E) \underset{\mathcal{W}(E)}{=} \sum_{\lambda \geqslant 1}^{N_L} \frac{\boldsymbol{d}_\lambda \boldsymbol{d}_\lambda^\mathsf{T}}{E - \mathcal{E}_\lambda} + \mathbf{Hol}_{\boldsymbol{D}}(E), \tag{36}$$

where $\mathbf{Hol}_{\boldsymbol{D}}(E)$ is a holomorphic (entire) part, and the definite residue widths $\boldsymbol{d}_\lambda$ are linked to the radioactive eigenvectors $\boldsymbol{v}_\lambda$ as

$$\boldsymbol{d}_\lambda = \frac{\boldsymbol{v}_\lambda}{\sqrt{\boldsymbol{v}_\lambda^\mathsf{T}\big(\frac{\partial \boldsymbol{D}^+}{\partial E}\big|_{E=\mathcal{E}_\lambda}\big)\boldsymbol{v}_\lambda}}, \tag{37}$$

where

$$\frac{\partial \boldsymbol{D}^+}{\partial E} = -\mathbb{I} + \boldsymbol{W} - \boldsymbol{\alpha}\frac{\partial \boldsymbol{L}}{\partial E}\boldsymbol{\alpha}^\mathsf{T}. \tag{38}$$

Conservation (24) thereupon entails the following link between the definite resonance widths $\alpha_{\lambda,c}$ and the residue widths of the Kapur-Peierls operator:

$$\boldsymbol{r}_\lambda = \boldsymbol{\alpha}^\mathsf{T}\boldsymbol{d}_\lambda. \tag{39}$$

This links our definite parametrization to the windowed multipole representation of R-matrix cross section established in [27], since one can construct the poles and residues expansion of analytically continued nuclear cross sections using these

Kapur-Peierls residue widths, by equating them in Eq. (39) of [27] to $\boldsymbol{r_\lambda} = \boldsymbol{\gamma}^\mathsf{T}\boldsymbol{a_\lambda} = \boldsymbol{\alpha}^\mathsf{T}\boldsymbol{d_\lambda}$.

Yet, because in the windowed multipole expansion we do not know the holomorphic parts explicitly—just as in Mittag-Leffler expansion (36)—and because we need to account for an infinity of poles in the Coulomb case, we say these expansions are local and incomplete. In contrast, our definite parametrization is global and complete: N_λ pairs of definite parameters $\{\mathcal{E}_\lambda, \alpha_{\lambda,c}\}$ will suffice to completely describe the scattering matrix (19) everywhere in the complex plane.

Applying differential equation (48) from Theorem 2 of [28] thereupon yields the following partial differential equation for the definite resonance widths:

$$\boldsymbol{a}\frac{\partial\,\boldsymbol{\alpha}^\mathsf{T}\boldsymbol{d_\lambda}}{\partial\boldsymbol{a}} + \left(\frac{1}{2}\mathbb{I} - \boldsymbol{L}\right)\boldsymbol{\alpha}^\mathsf{T}\boldsymbol{d_\lambda} \;=\; \boldsymbol{0}, \tag{40}$$

where $\boldsymbol{a} \triangleq \mathbf{diag}(a_c)$ is the diagonal matrix of channel radii, and $\boldsymbol{a}\frac{\partial\,\boldsymbol{\alpha}^\mathsf{T}\boldsymbol{d_\lambda}}{\partial\boldsymbol{a}}$ designates the channel-by-channel partial differential operator $a_c\frac{\partial[\boldsymbol{\alpha}^\mathsf{T}\boldsymbol{d_\lambda}]_{\lambda,c}}{\partial a_c}$.

Expression (40) dictates the transformation of the definite resonance widths $\alpha_{\lambda,c}$ under a change of channel radii $a_c \to a_c'$. Though we know these parameters, the definite levels $\mathcal{E}_\lambda$, as well as $\boldsymbol{L}$, and therefore the definite level matrix $\boldsymbol{D}$ and its derivatives from (20), as well as its residue widths $\boldsymbol{d_\lambda}$ from (37), transformation (40) nonetheless remains implicit, as it is essentially of the form

$$f\left(\boldsymbol{\alpha}, \frac{\partial\boldsymbol{\alpha}}{\partial\boldsymbol{a}}, \boldsymbol{v_\lambda}, \frac{\partial\boldsymbol{v_\lambda}}{\partial\boldsymbol{a}}\right) \;=\; 0$$

and the v_λ nullspace eigenvectors are subject to pseudonormalization (27) as well as their implicit constraint $\boldsymbol{D}^+(\mathcal{E}_\lambda)\boldsymbol{v_\lambda} = \boldsymbol{0}$.

F. Definite levels and nuclear resonances

Being the poles of the scattering matrix bestows upon the definite levels $\mathcal{E}_\lambda$ (or Siegert-Humblet radioactive states parameters) the important physical property that their real part $\mathrm{Re}[\mathcal{E}_\lambda]$ corresponds exactly to the resonances along the real energy line, and their imaginary part $\mathrm{Im}[\mathcal{E}_\lambda]$ to their widths.

Cross sections exhibit their resonance behavior as a linear combination of symmetric and antisymmetric Cauchy-Lorentz distributions:

$$\psi(x) \triangleq \frac{1}{1+x^2}, \quad \chi(x) \triangleq \frac{x}{1+x^2}. \tag{41}$$

These single-level Breit-Wigner profiles appear in the total cross section (7) through the Mittag-Leffler pole expansion of the transition matrix (akin to that of the definite level matrix (36) in Sec. III E, and we refer to articles [27,28] for further discussion of scattering matrix pole expansions):

$$\boldsymbol{T}(E) \underset{\mathcal{W}(E)}{=} \sum_{\lambda\geqslant 1}^{N_L} \frac{\boldsymbol{\tau_\lambda}\boldsymbol{\tau_\lambda}^\mathsf{T}}{E - \mathcal{E}_\lambda} + \mathbf{Hol}_{\boldsymbol{T}}(E), \tag{42}$$

where the transition matrix residue widths $\boldsymbol{\tau_\lambda}$ are linked to those $\boldsymbol{r_\lambda}$ of the Kapur-Peierls operator (39) according to Eq. (44) of [27]. Separating the definite levels in their real and imaginary parts,

$$\mathcal{E}_\lambda \;=\; \epsilon_\lambda - i\frac{\Gamma_\lambda}{2}, \tag{43}$$

and splitting the transition matrix residues into real and imaginary parts,

$$\boldsymbol{\tau_\lambda}\boldsymbol{\tau_\lambda}^\mathsf{T} \;=\; (\boldsymbol{a_\lambda} + i\boldsymbol{b_\lambda})\frac{\Gamma_\lambda}{2i}, \tag{44}$$

entails that the total cross section (7) can be expressed as the following linear combination of Cauchy-Lorentzian resonance profiles:

$$\sigma_c(E) \underset{\mathcal{W}(E)}{=} \frac{4\pi g_{J_c^\pi}}{|k_c(E)|^2}\,\mathrm{Re}\left[\sum_{\lambda\geqslant 1}^{N_L} a_\lambda^{cc}\,\psi(x_\lambda) \;+\; b_\lambda^{cc}\,\chi(x_\lambda) \;+\; \mathbf{Hol}_{\boldsymbol{T}}^{cc}(E)\right], \tag{45}$$

where the dimensionless variable x_λ is centered around the real part of definite energy $\epsilon_\lambda \triangleq \mathrm{Re}[\mathcal{E}_\lambda]$ with a width of size $\Gamma_\lambda \triangleq -2\,\mathrm{Im}[\mathcal{E}_\lambda]$ as

$$x_\lambda \;\triangleq\; \frac{E - \epsilon_\lambda}{\Gamma_\lambda/2}. \tag{46}$$

At each resonance, the symmetric profile $\psi(x_\lambda)$ peaks at ϵ_λ, while the antisymmetric profile $\chi(x_\lambda)$ is zero at ϵ_λ and has a peak and a dip at $x_\lambda = 1$ and $x_\lambda = -1$ (so that Γ_λ is the width of the resonance). Therefore, the definite levels $\mathcal{E}_\lambda$ describe exactly these resonances, with their real part corresponding to the resonance peak region (but not the exact value at which the peak occurs), and their imaginary part corresponding to the resonance width [thought the linear combination of symmetric and antisymmetric profiles (45) does not in general present peaks or zeros exactly at the ϵ_λ values, due to the linear combinations, or to the $\frac{1}{|k(E)|^2}$ general modulation factor of the cross sections]. The definite levels $\mathcal{E}_\lambda$ are therefore the natural physical quantities to describe the resonances.

Note that expansion (45) is but the windowed multipole representation established in [27], and the same approach can thereupon be taken to write the elastic scattering matrix (1) using the conjugate continuation described in Sec. II D of [27] (see Sec. II E for more explanations), yielding a similar form:

$$\sigma_{cc'}(E) \underset{\mathcal{W}(E)}{=} \frac{4\pi g_{J_c^\pi}}{|k_c(E)|^2}\,\mathrm{Re}\left[\sum_{\lambda\geqslant 1}^{N_L} \widetilde{a_\lambda^{cc'}}\,\psi(x_\lambda) \;+\; \widetilde{b_\lambda^{cc'}}\,\chi(x_\lambda) \;+\; \mathbf{Hol}_{\boldsymbol{T}}^{cc}(E)\right], \tag{47}$$

where $\widetilde{a_\lambda^{cc'}}$ and $\widetilde{b_\lambda^{cc'}}$ are real and imaginary parts of the matrix elements of (with $\circ$ designating the elementwise Hadamard matrix product)

$$\boldsymbol{\tau_\lambda}\boldsymbol{\tau_\lambda}^\mathsf{T} \circ [\boldsymbol{T}(\mathcal{E}_\lambda^*)]^* \;=\; (\widetilde{\boldsymbol{a_\lambda}} + i\widetilde{\boldsymbol{b_\lambda}})\frac{\Gamma_\lambda}{2i}. \tag{48}$$

We just showed how the poles of the scattering matrix are natural variables to describe the resonance profiles, even though we do not know the explicit set of constraints on

the definite parameters. However, some general properties are known, since fundamental physics principles constrain the poles of the scattering matrix to specific symmetries. Unitarity imposes specular symmetry along the imaginary wave number axis: if k_c is a pole of the scattering matrix, then so is $-k_c*$, and Eden and Taylor's generalized such relations to all channels and sheets of mappings (15) (cf. the generalized unitarity relation (2.16) of [38]). Moreover, causality entails that the scattering matrix poles are usually either *radioactive states* (or *resonance states*), when they dwell on the unphysical sheet (defined as $\mathrm{Im}[k_c] < 0$), or *bound states* when they dwell on the physical sheet (defined as $\mathrm{Im}[k_c] > 0$), in which case they are restricted to the positive imaginary axis (i.e., $\mathrm{Re}[k_c] = 0$) (cf. Sec. IX 2 d in [2]).

In the Wigner-Eisenbud R-matrix parametrization, real resonance energies E_λ and boundary conditions B_c preserve unitarity. However, the Reich-Moore approximation in effect introduces complex resonance energies (10), which can violate the unitarity of the scattering matrix. We observe this breaking of symmetry in the case of xenon isotope ^{134}Xe, spin-parity group $J^\pi = 1/2^{(-)}$, where the scattering matrix poles (definite levels documented in Table I) do not exactly respect specular symmetry, and the bound state is close to but not exactly on the imaginary axis.

G. Nuclear data evaluations in definite parametrization

We showed how the definite levels $\mathcal{E}_\lambda$ are the physically natural variables for describing the resonances. However, their constraints are implicit (as discussed in Sec. III E), which entails one cannot perform a nuclear data evaluation directly with the definite parameters — fitting whichever definite levels $\mathcal{E}_\lambda$ and definite widths $\alpha_{\lambda,c}$ that best match the observed data.

This is because we do not know explicitly the set of constraints in the complex plane within which it is physically admissible for the definite parameters to evolve. The traditional Wigner-Eisenbud R-matrix parameters are admissible as long as they are real (that is their space of constraints). In contrast, the definite parameters are only admissible as long as they satisfy (26) and (28). Therefore, in order to guarantee the equivalence between the Wigner-Eisenbud and the definite parametrization, one must first perform the nuclear data evaluation with Wigner-Eisenbud parameters, and then transform the latter into definite parameters as specified in Sec. III B. Only then will the definite parametrization defined in Sec. III A be correct.

Despite this major drawback, there are nonetheless clear benefits to specifying the definite parameters of a nuclear data evaluation, as their invariance properties guarantee a physics-based unified framework within which to compare evaluations performed with different boundary conditions or channel radii. In other words, if two evaluations of the same nuclear cross section are done with different boundary conditions B_c and channel radii a_c, they will yield different Wigner-Eisenbud R-matrix parameters $\{E_\lambda, \gamma_{\lambda,c}\}$. Yet, both can then be transformed into our definite R-matrix parameters $\{\mathcal{E}_\lambda, \alpha_{\lambda,c}\}$, which are now all boundary conditions B_c independent, and—though the set of definite resonance widths $\alpha_{\lambda,c}$ will depend on the choice of channel radii a_c according to implicit relation (40)—both evaluations will yield the same set of definite levels $\mathcal{E}_\lambda$, independent of the choice of channel radii a_c. This invariance makes of the definite parameters $\{\mathcal{E}_\lambda, \alpha_{\lambda,c}\}$ the most natural and convenient—they are universal (invariant physical quantities) and have no boundary conditions B_c, which entails fewer parameters—set of R-matrix parameters with which to completely describe and document nuclear cross sections in future standard evaluated nuclear data libraries (ENDF [5], JEFF [6], BROND [7], JENDL [8], CENDL [9], TENDL [10,11]).

Concerning evaluations, we end with a note on how to account for the tail contributions of negative energy bound states, or high-energy resonances, sometimes called "background cross section terms." As tail effects, these can be difficult to fit, which is why evaluators have traditionally resorted to either (a) adding so-called 'dummy resonances' away from the energy region (far-off bound or resonance states) (see SAMMY format LRF = 3 [39]), or (b) recently introducing a somewhat *ad hoc* functional fit (in SAMMY format LRF = 7, Sec. II B 1 d of manual [39]). Though we appreciate the honesty of approach (b), which acknowledges where we are curve-fitting versus where we are evaluating (resolving resonances and thresholds), we nonetheless believe that approach (a) is more physically appropriate in that these tail effects are the result of true resonances or bound states, of which there may be an infinite number, sometimes very far away from the energy region being evaluated. Though we may not be able to (nor seek to) accurately resolve all these resonances and bound states, fitting them with pseudoresonances that account well enough for their tail effects is just as universal an approximation (see Runge's theorem) as fitting these tails with other *ad hoc* functional forms, which do not fall within the existing framework of R-matrix theory. Moreover, the Mittag-Leffler expansions of R-matrix cross sections, established in the windowed multipole representation [27], equivalent to herein established Eqs. (45) and (47), in fact show that the holomorphic part of R-matrix cross sections (as well as the infinity of poles and residues) are exactly and completely described by both the Wigner-Eisenbud R-matrix parametrization (8), or equivalently our definite parametrization of R-matrix theory (19), using only N_λ definite levels $\mathcal{E}_\lambda$. Though the number N_λ is *a priori* unknown by the evaluator, one can continue to add resonances until the fit is sufficiently accurate for our measurements' uncertainty. If the difficulty lies in numerically fitting the tails from the experimental data, we point to advanced new methods and algorithms—for instance [40–45]—that could help directly find the definite levels $\mathcal{E}_\lambda$, poles of the scattering matrix. Some of these methods have been recently used with some success to establish the Windowed Multipole Library (see the last paragraph of Sec. II E 3 in [27], or [46,47]).

This points to an additional major advantage of our definite parametrization of R-matrix theory: documenting the definite parameters ($\mathcal{E}_\lambda$ levels and $\alpha_{\lambda,c}$ widths) in future standard nuclear data libraries would somewhat greatly simplify the recording of and conversion to the windowed multipole representation established in [27]. This is because the N_λ principal definite levels $\mathcal{E}_\lambda$ provide a unified set of multipoles p_j across

all windows (through their square root, as of Eq. (47) in [27]). One can then compute their residues using the contour integrals Eq. (83) and Eq. (84) in [27], so that the Windowed Multipole Library [27,48,49] can consist of a unified global list of principal poles and residues, and then a set of energy windows. For each window, we can then document: a subset of indices indicating which of the N_λ principal definite levels $\mathcal{E}_\lambda$ (and their corresponding residues) are used in the window; and a set of Laurent expansion coefficients (background terms).

H. Remarks on an alternative, non-invariant, definite parameterization

Our definite parametrization, defined in Sec. III A, rested upon the assumption that the $\boldsymbol{v_\lambda}$ radioactive eigenvectors of (26) are pseudonormalizable as in (27). Though we argued that making this assumption is unlikely to pose a problem in practice, it is nonetheless possible to define another, similar parametrization which does not require this assumption. This can be achieved in a similar fashion by defining an alternative definite level matrix $\widetilde{\boldsymbol{D}}$ as the pseudoinverse:

$$\widetilde{\boldsymbol{D}}(E) \triangleq [\widetilde{\boldsymbol{V}}^\dagger \boldsymbol{A^{-1}}(E)\widetilde{\boldsymbol{V}}]^+,$$

where the $\widetilde{\boldsymbol{V}}$ matrix is now composed of the size-N_c column eigenvectors, $\widetilde{\boldsymbol{V}} \triangleq [\widetilde{\boldsymbol{v_1}}, \ldots, \widetilde{\boldsymbol{v_\lambda}}, \ldots, \widetilde{\boldsymbol{v_{N_L}}}]$, solutions to the radioactive states generalized eigenproblem (26), but now properly normalized with their Hermitian conjugate $[\,\cdot\,]^\dagger$ as

$$\widetilde{\boldsymbol{v_\lambda}}^\dagger \widetilde{\boldsymbol{v_\lambda}} = 1.$$

We can then define the alternative definite parameters as

$$\widetilde{\boldsymbol{\alpha}} \triangleq \widetilde{\boldsymbol{V}}^\dagger \boldsymbol{\gamma}, \quad \widetilde{\boldsymbol{\beta}} \triangleq \widetilde{\boldsymbol{V}}^\dagger \sqrt{\boldsymbol{\Gamma_\gamma}},$$

where $\sqrt{\boldsymbol{\Gamma_\gamma}} \triangleq \mathbf{diag}_\lambda(\sqrt{\Gamma_{\lambda,\gamma}})$ is the diagonal matrix of the eliminated capture widths in the Reich-Moore formalism (10).

Through this construction, the alternative definite level matrix $\widetilde{\boldsymbol{D}}$ now is explicitly parametrized as

$$\widetilde{\boldsymbol{D}}^+ = \widetilde{\boldsymbol{Q}} - E\widetilde{\boldsymbol{W}} - \widetilde{\boldsymbol{\alpha}}\boldsymbol{L}(E)\widetilde{\boldsymbol{\alpha}}^\dagger$$

with

$$\widetilde{Q}_{\lambda\mu} = \sum_{c=1}^{N_c} \frac{\widetilde{\alpha}_{\lambda,c}(L_c(\mathcal{E}_\mu)\mathcal{E}_\lambda^* - L_c(\mathcal{E}_\lambda)^*\mathcal{E}_\mu)\widetilde{\alpha}^*_{\mu,c}}{\mathcal{E}_\lambda^* - \mathcal{E}_\mu} + i\,\mathcal{E}_\mu \sum_{\eta=1}^{N_\lambda} \frac{\widetilde{\beta}_{\lambda,\eta}\widetilde{\beta}^*_{\mu,\eta}}{\mathcal{E}_\lambda^* - \mathcal{E}_\mu}$$

and

$$\widetilde{W}_{\lambda\mu} = \sum_{c=1}^{N_c} \frac{\widetilde{\alpha}_{\lambda,c}(L_c(\mathcal{E}_\mu) - L_c(\mathcal{E}_\lambda)^*)\widetilde{\alpha}^*_{\mu,c}}{\mathcal{E}_\lambda^* - \mathcal{E}_\mu} + i \sum_{\eta=1}^{N_\lambda} \frac{\widetilde{\beta}_{\lambda,\eta}\widetilde{\beta}^*_{\mu,\eta}}{\mathcal{E}_\lambda^* - \mathcal{E}_\mu}.$$

This alternative parametrization guarantees

$$\widetilde{\boldsymbol{\alpha}}^\dagger \widetilde{\boldsymbol{D}} \widetilde{\boldsymbol{\alpha}} = \boldsymbol{\gamma}^\mathsf{T} \boldsymbol{A} \boldsymbol{\gamma}$$

so that the scattering matrix expression

$$\boldsymbol{U} = \boldsymbol{O}^{-1}\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}\widetilde{\boldsymbol{\alpha}}^\dagger\widetilde{\boldsymbol{D}}\widetilde{\boldsymbol{\alpha}}\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}$$

is also a complete alternative parametrization of R-matrix theory.

Though similar to our definite parametrization of Sec. III A, there are three major differences in this alternative parametrization:

(i) It does not require assuming that pseudonormalization (27) is possible (Hermitian normalization $\widetilde{\boldsymbol{v_\lambda}}^\dagger \widetilde{\boldsymbol{v_\lambda}} = 1$ is always possible).
(ii) It presents additional alternative definite capture widths $\widetilde{\beta}_{\lambda,\mu}$ for each pair of levels.
(iii) It is no longer invariant with a change of arbitrary boundary condition $\boldsymbol{B} \to \boldsymbol{B'}$, because the Hermitian conjugates in Sec. III H entail that the proof of invariance of Sec. III D is no longer valid.

While the presence of a new nondiagonal matrix of alternative eliminated capture widths $\widetilde{\boldsymbol{\beta}}$ is interesting in that it can be interpreted as an analog of the diagonal matrix $\sqrt{\boldsymbol{\Gamma_\gamma}}$ of eliminated capture widths in the Reich-Moore formalism (10), and that the $\widetilde{\beta}_{\lambda,\mu}$ are therefore null in the absence of these Reich-Moore parameters, it is nonetheless relatively cumbersome and would induce a heavy increase in the number of evaluated parameters needed to parametrize the same cross section. Moreover, the fact that this alternative parametrization is not invariant under a change of boundary parameters $\boldsymbol{B} \to \boldsymbol{B'}$ defeats the purpose of a definite parametrization, and is therefore prohibitive. Hence we do not propose this parametrization as our definite, complete, invariant, parametrization of R-matrix theory.

However, we still expanded on it for two reasons: (1) In a general way, this is a clear example of how complex symmetry (and not Hermitian conjugacy) is the physically and mathematically natural form of symmetry for scattering problems. (2) In a more particular fashion, this Hermitian approach is the one we took in Sec. IV A of article [14], which is therefore not invariant under a change of boundary conditions $\boldsymbol{B} \to \boldsymbol{B'}$. Though we did not explicitly claim that such generalization to the Reich-Moore formalism of the Brune parametrization was invariant to a change of boundary condition $\boldsymbol{B} \to \boldsymbol{B'}$, we now believe that it is not, so that a more proper generalization of the Brune parameters ought not be made as in Sec. IV A of article [14], but rather as we here did in Sec. III A, by replacing the $\boldsymbol{L}(E)$ operator with the shift operator $\boldsymbol{S}(E)$, which would guarantee invariance to a change of boundary parameters $\boldsymbol{B} \to \boldsymbol{B'}$ (but not to a change of channel radii), as per Sec. III D.

IV. EVIDENCE ON XENON 134

In the wake of our xenon trilogy on R-matrix pole parametrizations [14,27,28], we here present evidence of the definite parametrization in xenon isotope ^{134}Xe, spin-parity group $J^\pi = 1/2^{(-)}$, which presents two p-waves resonances. There, we observe the different physical phenomena and properties described in Sec. III.

The ^{134}Xe evaluation in the ENDF/B-VIII.0 [5] nuclear data library uses the Reich-Moore formalism in that there is only one explicitly treated channel (neutron elastic scattering

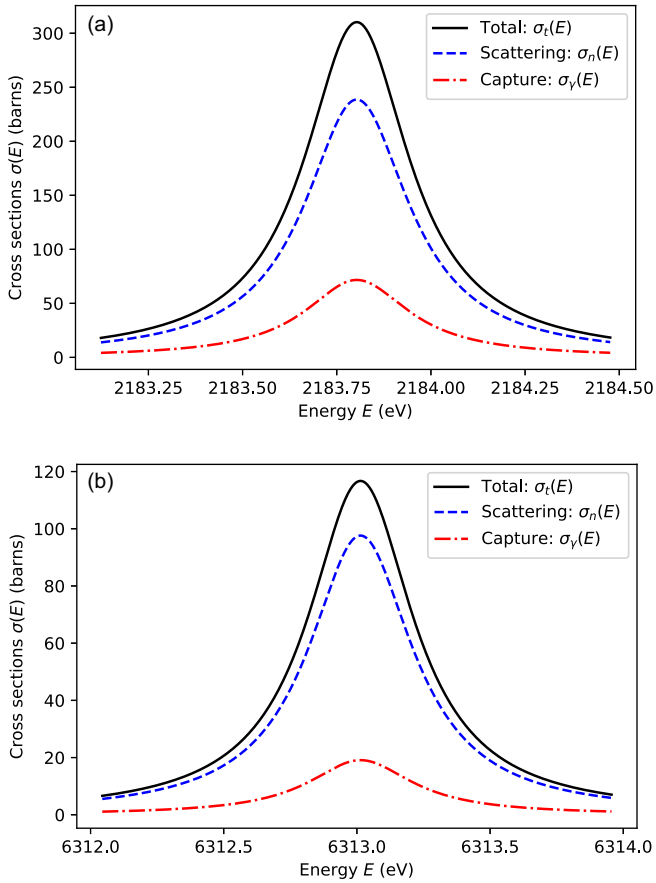

FIG. 2. Partial cross sections of ^{134}Xe, spin-parity group $J^\pi = 1/2^{(-)}$. (a) First p-wave resonance. (b) Second p-wave resonance. The two p-wave resonances are computed from the scattering matrix $\boldsymbol{U}(E)$ using either the definite parameters from Table I in expression (19) or the Wigner-Eisenbud R-matrix parameters from Table I in expression (8) using the Reich-Moore level-matrix (11), both yielding identical results. Total cross section is from (7), elastic scattering cross section from (1), and eliminated γ-capture cross section from the difference of the two.

$N_c = 1$), and the γ-capture channel is eliminated through capture widths $\Gamma_{\lambda,\gamma}$ as in (10). For generality, we thus decide to use the full Reich-Moore level matrix (11), instead of the simplified multilevel Breit-Wigner (MLBW) one used for this specific ENDF evaluation (see Eq. (22) of [27]).

First, we construct all the $N_L \times N_c$ definite parameters, converting them from the Wigner-Eisenbud R-matrix ones as specified in Sec. III B, and document them here in Table I. The definite levels $\mathcal{E}_\lambda$—found by solving (26)—are the radioactive state poles documented in Table I of [28], from which the definite resonance widths $\alpha_{\lambda,c}$ are constructed using (28). As predicted by (31), one can see that the number of definite levels is here $N_L = 5$, as there are $N_\lambda = 2$ resonance energies for this sole p-wave channel (so that $\ell_c = 1$), and zero is the only threshold energy (so that $N_{E_{T_c} \neq E_{T_{c'}}} = 1$). To find the $\pm$ sheet of energy–wave-number mapping (17) on which the definite levels dwell, we unfolded the Riemann surface through change of variable $z^2 = E$ and solved for the radioactive eigenproblem (26) in z space. The results are

TABLE II. Alternative, noninvariant, definite parameters—definite levels $\mathcal{E}_\lambda$ (Siegert-Humblet radioactive state resonance energies, poles of the scattering matrix) from Table I, and alternative definite resonance $\widetilde{\alpha}_{\lambda,c}$ and eliminated capture $\widetilde{\beta}_{\lambda,\mu}$ widths of the alternative definite parametrization of Sec. III H—of the two p-wave resonances of ^{134}Xe, spin-parity group $J^\pi = 1/2^{(-)}$, converted from the Wigner-Eisenbud R-matrix parameters reported in ENDF/B-VIII.0 (MLBW evaluation) using the Reich-Moore level matrix (11) in R-matrix parametrization (8), as per Table I.

Alternative definite, noninvariant parameters (rounded to 5 digits)	
Alternative definite resonance widths $\widetilde{\alpha}_{\lambda,c}$ from Sec. III H ($\sqrt{\text{eV}}$)	Alternative definite eliminated widths $\widetilde{\beta}_{\lambda,\mu}$ from Sec. III H (dimensionless)
$2.8812 \times 10^{+1}$ $+i2.7712 \times 10^{-9}$	$\begin{bmatrix} 2.4389 \times 10^{-1} \\ 1.3608 \times 10^{-1} \\ +i5.4857 \times 10^{-11} \end{bmatrix}$
$2.5126 \times 10^{+1}$ $+i2.4873 \times 10^{-4}$	$\begin{bmatrix} 2.7928 \times 10^{-1} \\ 8.3405 \times 10^{-5} \\ +i4.9238 \times 10^{-6} \end{bmatrix}$
$2.5126 \times 10^{+1}$ $-i2.4858 \times 10^{-4}$	$\begin{bmatrix} 2.7928 \times 10^{-1} \\ 8.3406 \times 10^{-5} \\ -i4.9208 \times 10^{-6} \end{bmatrix}$
$1.4087 \times 10^{+1}$ $-i2.1607 \times 10^{-3}$	$\begin{bmatrix} -2.3937 \times 10^{-4} \\ -i2.40207 \times 10^{-5} \\ 2.7928 \times 10^{-1} \end{bmatrix}$
$1.4087 \times 10^{+1}$ $+i2.1604 \times 10^{-3}$	$\begin{bmatrix} -2.3937 \times 10^{-4} \\ +i2.4018 \times 10^{-5} \\ 2.7928 \times 10^{-1} \end{bmatrix}$

documented in Table I. Note that, as a nonlinear generalized eigenproblem, solving the radioactive states problem (26) can be numerically arduous, and we refer for further discussion to the last paragraph of Sec. II C in [28], or to Secs. II E 3 and II F 1 in [27].

Then, we computed the scattering matrix either with the traditional Wigner-Eisenbud R-matrix parametrization (8), or with the definite parametrization (19), verifying they yield identical results, which confirms our definite parametrization is indeed an equivalent parametrization of R-matrix theory, with the benefits of being definite, complete, and invariant. The surface of the scattering matrix modulus $|\boldsymbol{U}|(z)$ is plotted in Fig. 1. There, the $N_L = 5$ different poles (definite levels $\mathcal{E}_\lambda$) of Table I are clearly visible: two for each resonance energy E_λ, one "resonant pole" on the physical $\{+\}$ sheet (on the positive side of the real z axis), and another "shadow pole" on the nonphysical $\{-\}$ sheet (on the negative side of the real z axis) of mapping (17). The fifth pole (on the first line of Table I), which is introduced by the outer region $\boldsymbol{L}(\boldsymbol{\rho})$ operator of the p wave (angular momentum $\ell = 1$), is also clearly visible: this pole is far away from all the resonances, and is much farther from the real z axis (or much closer to the real E axis) than the other poles, as well as being considerably wider (larger residue). This "outer pole" is not the shadow of a resonant pole (and dwells on the physical $\{+\}$ sheet), but instead is representative of another class of poles, which we could name "angular momenta scattering poles."

Here, we empirically confirm the choice of definite parameters result of Sec. III C, whereby, out of the five definite parameters sets $\{\mathcal{E}_\lambda, \alpha_{\lambda,c}\}$ in Table I, one can choose any two, three, four, or five, and use only these to compute the definite level matrix $\boldsymbol{D}$ through pseudoinverse definition (20), and hence the scattering matrix $\boldsymbol{U}(E)$ through (19). Somewhat remarkably, this will always yield the exact same scattering matrix, with all five poles visible in Fig. 1, thereby also guaranteeing that any choice of at least two of the definite parameters will result in the exact same cross sections of Fig. 2.

Since they are equivalent and yield the same scattering matrix, the definite and the Wigner-Eisenbud parametrizations of R-matrix theory yield the exact same cross sections. The ^{134}Xe p-wave spin-parity $J^\pi = 1/2^{(-)}$ total cross section is computed using Eq. (7), and the elastic scattering cross section using (1), so that the difference of the two yields the eliminated γ-capture cross section. These three different partial cross sections have two resonances (circa 2183.8 eV and 6313.0 eV), which are here reported in Fig. 2. The elastic scattering cross section (1), depicted as a dotted blue line in Fig. 2, is linked through (3) to the scattering matrix modulus along the real z axis, rendered as a red line on the surfaces of Figs. 1 (see Fig. 1(c) zoom).

For completeness, we end by reporting in Table II the alternative, noninvariant parameters discussed in Sec. III H. As discussed therein, these alternative parameters are analogous to the ones we proposed in Table VI of [14], and we here argue they are not invariant to change of boundary conditions $\boldsymbol{B} \rightarrow \boldsymbol{B}'$. We thus do not recommend using either of these, but instead recommend the proper definite parameters of Table I, and define the generalized Brune parameters for Reich-Moore formalism as we here do in Secs. III A and III B, only replacing the $\boldsymbol{L}$ operator with the shift operator $\boldsymbol{S}$.

V. CONCLUSION

We here establish a definite parametrization of R-matrix theory, which completely describes the scattering matrix (hence also the cross sections), using the physical scattering matrix poles $\mathcal{E}_\lambda$, but only as many as there are Wigner-Eisenbud resonance levels E_λ. This sets a one-to-one correspondence between the traditional Wigner-Eisenbud and our definite parametrization of R-matrix theory.

As major benefits, our definite parametrization is invariant to (and does not require the prescription of) arbitrary boundary conditions B_c (contrary to the traditional Wigner-Eisenbud parametrization of R-matrix theory). Moreover, being poles of the scattering matrix, the definite levels $\mathcal{E}_\lambda$ are now complex and invariant with respect to changes in channel radius a_c (contrary to the alternative Brune parametrization). They also correspond to nuclear cross sections resonances, describing their peaks and widths exactly.

In a general framework that encompasses the Reich-Moore formalism, we show how to convert the traditional Wigner-Eisenbud R-matrix parameters into our new definite parameters, composed of the definite levels $\mathcal{E}_\lambda$ and Ducru definite widths $\alpha_{\lambda,c}$ (which are now all complex numbers). As a result, this novel definite parametrization of R-matrix theory can be equivalently used as a new, complete, and invariant format for nuclear data evaluations.

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