Scattering matrix pole expansions for complex wave numbers in *R*-matrix theory

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In this followup article to Ducru *et al.* [Phys. Rev. C **103**, 064608 (2021)], we establish new results on scattering matrix pole expansions for complex wave numbers in *R*-matrix theory. In the past, two branches of theoretical formalisms emerged to describe the scattering matrix in nuclear physics: *R*-matrix theory and pole expansions. The two have been quite isolated from one another. Recently, our study of Brune's alternative parametrization of *R*-matrix theory has shown the need to extend the scattering matrix (and the underlying *R*-matrix operators) to complex wave numbers. Two competing ways of doing so have emerged from a historical ambiguity in the definitions of the shift $\boldsymbol{S}$ and penetration $\boldsymbol{P}$ functions: the legacy Lane and Thomas's "force closure" approach versus analytic continuation (which is the standard in mathematical physics). The *R*-matrix community has not yet come to a consensus as to which to adopt for evaluations in standard nuclear data libraries, such as ENDF. In this article, we argue in favor of analytic continuation of *R*-matrix operators. We bridge *R*-matrix theory with the Humblet-Rosenfeld pole expansions, and discover new properties of the Siegert-Humblet radioactive poles and widths, including their invariance properties to changes in channel radii a_c. We then show that analytic continuation of *R*-matrix operators preserves important physical and mathematical properties of the scattering matrix—canceling spurious poles and guaranteeing generalized unitarity—while still being able to close channels below thresholds.

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I. INTRODUCTION

Myriad nuclear interactions have been modeled with *R*-matrix theory, with applications to many branches of nuclear physics, from nuclear simulation, radiation transport, astrophysics, and cosmology, and extending to particle physics or atomistic and molecular simulation [1–8]. Our current nuclear data libraries are based on *R*-matrix evaluations (ENDF [9], JEFF [10], BROND [11], JENDL [12], CENDL [13], TENDL [14,15]). The *R*-matrix scattering model takes different incoming particle waves and lets them interact through a given Hamiltonian to produce different possible outcomes. *R*-matrix theory studies the particular two-body-in–two-body-out model of this scattering event, with the fundamental assumption that the total Hamiltonian is the superposition of a short-range, interior Hamiltonian, which is null after a given channel radius a_c, and a long-range, exterior Hamiltonian, which is well known (free particles or Coulomb potential, for instance) [2,16–18]. *R*-matrix theory can then parametrize the energy dependence of the scattering matrix in different ways. The Wigner-Eisenbud parametrization is the historical standard, because its parameters are real and well defined, though some are arbitrary (the channel radius a_c and the boundary condition B_c). To remove this dependence on an arbitrary boundary condition B_c, the nuclear community has recently been considering shifting nuclear data libraries to an alternative parametrization of *R*-matrix theory [19–22].

In parallel, there is vast literature in mathematical physics and nuclear physics on pole expansions of the scattering matrix [23–27], starting with the well-known developments by Humblet and Rosenfeld [28–35].

This article follows [22], precedes [36], and is thus the second in our trilogy on pole parametrizations of *R*-matrix theory (see Supplemental Material of Ref. [22]). In Sec. II, we show how the Siegert-Humblet expansion into radioactive states is the link between *R*-matrix theory and the scattering matrix pole expansions of Humblet and Rosenfeld. In the process, we unveil new relations between the radioactive poles and residues and the alternative parametrization of *R*-matrix theory, and establish for the first time the number of radioac-

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tive poles in wave-number space (Theorem 1) along with their branch structure. Section III investigates the invariance properties of Siegert-Humblet radioactive state parameters to a change in channel radius a_c. We demonstrate in Theorem 2 that invariance of the scattering matrix to a_c sets a partial differential equation on the Kapur-Peierls operator $\boldsymbol{R}_L$, which in turn enables us to derive explicit transformations of the Siegert-Humblet radioactive widths $\{r_{j,c}\}$ under a change of channel radius a_c. Section IV considers the continuation of the scattering matrix to complex wave numbers in R-matrix theory. We establish several new results. We show that the legacy of Lane and Thomas to force-close channels below threshold not only breaks the analytic properties of the scattering matrix but also introduces nonphysical spurious poles. Yet, we prove that these spurious poles are canceled out if one performs analytic continuation of R-matrix operators instead (Theorem 3). We also show that this analytic continuation of R-matrix operators enforces the generalized unitarity conditions described by Eden and Taylor [37] (Theorem 4). Finally, in the case of massive particles, we propose a solution to the conundrum of how to close the channels below thresholds, by invoking both a quantum tunneling argument, whereby the transmission matrix is evanescent below threshold (Theorem 5), and a physical argument based on the definition of the cross section as the ratio of probability currents (Theorem 6). All these results make us argue that, contrary to what Lane and Thomas prescribed [2], the R-matrix parametrization should be analytically continued to complex wave numbers $k_c \in \mathbb{C}$. These considerations have practical implications on R-matrix evaluation codes, such as EDA [38,39], SAMMY [40], and AZURE [41], used to build our nuclear data libraries: ENDF [9], JEFF [10], BROND [11], JENDL [12], CENDL [13], TENDL [14,15]). We thus call for analytic continuation of R-matrix operators to become the new standard for nuclear cross section evaluations.

II. SIEGERT-HUMBLET POLE EXPANSION IN RADIOACTIVE STATES

We here establish new R-matrix theory results concerning the Siegert-Humblet expansion into radioactive states (cf. Sec. IX.2.c–e, pp. 297–298, in Ref. [2]). These *radioactive state parameters* express the energy dependence of the scattering matrix into a simple sum of poles and residues. We show this constitutes the link between R-matrix theory and the scattering matrix pole expansions of Humblet and Rosenfeld [28–35] (Sec. II F). In the wake, we show how to obtain the radioactive state parameters (Sec. II A), link them to the Brune alternative parametrization (Sec. II B), reveal their branch structure (Theorem 1, Sec. II C), which emerges from the wave number energy mapping (1),

$$\rho_c(E) \longleftrightarrow E, \tag{1}$$

where $\rho_c \triangleq a_c k_c$ is the dimensionless wave-number variable $\boldsymbol{\rho} \triangleq \mathbf{diag}(\rho_c)$, a_c is the arbitrary channel radius, and $k_c(E)$ is the wave number of channel c, which is linked to the energy E of the system (eigenvalue of the Hamiltonian of the Schödinger equation) as explained in Sec. II.A of Ref. [22].

A. Definition of Siegert and Humblet parametrization

Following the notation of Ref. [22] (to which we refer for further explanations), we here recall the essential relation expressing the scattering matrix $\boldsymbol{U}$ as a function of R-matrix operators:

$$\boldsymbol{U} = \boldsymbol{O}^{-1}\boldsymbol{I} + 2\mathrm{i}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}\boldsymbol{R}_L\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}, \tag{2}$$

where $\boldsymbol{I}$ and $\boldsymbol{O}$ are the incoming and outgoing wave functions, which are subject to the following Wronksian condition: For all channel c, $w_c \triangleq O_c^{(1)}I_c - I_c^{(1)}O_c = 2\mathrm{i}$, or with identity matrix $\mathbb{I}$ (expression (7) in Ref. [22]) and denoting $[\,\cdot\,]^{(1)}$ the diagonal channel c derivative with respect to ρ_c

$$\boldsymbol{w} \triangleq \boldsymbol{O}^{(1)}\boldsymbol{I} - \boldsymbol{I}^{(1)}\boldsymbol{O} = 2\mathrm{i}\mathbb{I} \tag{3}$$

and where $\boldsymbol{R}_L$ is the *Kapur-Peierls operator*, defined as (see Eq. (20) in Sec. II.D of Ref. [22])

$$\boldsymbol{R}_L \triangleq [\mathbb{I} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B})]^{-1}\boldsymbol{R} = \boldsymbol{\gamma}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{\gamma}. \tag{4}$$

This Kapur-Peierls $\boldsymbol{R}_L$ operator is at the heart of the Siegert-Humblet parametrization, and its study is a core part of this article. The Kapur-Peierls operator $\boldsymbol{R}_L$ is a function of the Wigner-Eisenbud R-matrix $\boldsymbol{R}$, parametrized by the *resonance parameters* [energies $\boldsymbol{e} \triangleq \mathbf{diag}(E_\lambda)$ and widths $\boldsymbol{\gamma} \triangleq \mathbf{mat}(\gamma_{\lambda,c})$]

$$\boldsymbol{R}(E) \triangleq \boldsymbol{\gamma}^{\mathsf{T}}(\boldsymbol{e} - E\,\mathbb{I})^{-1}\boldsymbol{\gamma} \tag{5}$$

as well as the arbitrary boundary condition $\boldsymbol{B} \triangleq \mathbf{diag}(B_c)$ and the reduced logarithmic derivative of the outgoing wave function $\boldsymbol{L} \triangleq \mathbf{diag}(L_c)$, defined as (cf. Sec. II.B of Ref. [22])

$$L_c(\rho_c) \triangleq \frac{\rho_c}{O_c}\frac{\partial O_c}{\partial \rho_c} \tag{6}$$

and which admits the following Mittag-Leffler pole expansion (Theorem 1 of Sec. II.B of Ref. [22]),

$$\frac{L_c(\rho)}{\rho} = \frac{-\ell}{\rho} + \mathrm{i} + \sum_{n\geqslant 1}\frac{1}{\rho - \omega_n}, \tag{7}$$

where $\{\omega_n\}$ are the roots of the $O_c(\rho)$ outgoing wave functions: $\forall n,\ O_c(\omega_n) = 0$ (reported in Table II of Ref. [22] for neutral particles).

Equivalently, the Kapur-Peierls operator $\boldsymbol{R}_L$ can be expressed with the level matrix $\boldsymbol{A}$ (see Eqs. (17) and (18) in Sec. II.C of Ref. [22]):

$$\boldsymbol{A}^{-1} \triangleq \boldsymbol{e} - E\mathbb{I} - \boldsymbol{\gamma}(\boldsymbol{L} - \boldsymbol{B})\boldsymbol{\gamma}^{\mathsf{T}}. \tag{8}$$

All these R-matrix operators are functions of the wave numbers $k_c(E)$ [or their corresponding dimensionless wave-number variable $\boldsymbol{\rho} \triangleq \mathbf{diag}(\rho_c)$]. The Siegert-Humblet pole expansion in radioactive states consists of analytically continuing the Kapur-Peierls $\boldsymbol{R}_L$ operator to complex wave numbers $k_c \in \mathbb{C}$, thereby becoming a locally meromorphic operator. The poles of this meromorphic operator can be assumed to have a Laurent expansion of order one (i.e., simple poles), as we will discuss in Sec. IV C. Since the Kapur-Peierls $\boldsymbol{R}_L$ operator is complex symmetric, its residues at any given pole value $\mathcal{E}_j \in \mathbb{C}$ are also complex symmetric. For nondegenerate eigenvalues $\mathcal{E}_j \in \mathbb{C}$, the corresponding residues are rank 1 and expressed as $\boldsymbol{r}_j\boldsymbol{r}_j^{\mathsf{T}}$, while for degenerate eigenvalues $\mathcal{E}_j \in \mathbb{C}$

of multiplicity M_j, the corresponding residues are rank M_j and expressed as $\sum_{m=1}^{M_j} \boldsymbol{r}_j^m \boldsymbol{r}_j^{m\mathsf{T}}$. On a given domain, the Mittag-Leffler theorem [42,43] then states that $\boldsymbol{R}_L$ locally takes the form, in the vicinity $\mathcal{W}(E)$ (neighborhood) of any complex energy $E \in \mathbb{C}$ away from the branch points (threshold energies E_{T_c}) of mapping (1), of a sum of poles and residues and a holomorphic entire part $\mathbf{Hol}_{\boldsymbol{R}_L}(E)$:

$$\boldsymbol{R}_L(E) \underset{\mathcal{W}(E)}{=} \sum_{j\geqslant 1} \frac{\sum_{m=1}^{M_j} \boldsymbol{r}_j^m \boldsymbol{r}_j^{m\mathsf{T}}}{E-\mathcal{E}_j} + \mathbf{Hol}_{\boldsymbol{R}_L}(E), \tag{9}$$

or, in the particular (but most common) case where $\mathcal{E}_j$ is a nondegenerate eigenvalue (with multiplicity $M_j = 1$),

$$\boldsymbol{R}_L(E) \underset{\mathcal{W}(E)}{=} \sum_{j\geqslant 1} \frac{\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}}}{E-\mathcal{E}_j} + \mathbf{Hol}_{\boldsymbol{R}_L}(E). \tag{10}$$

This is the Siegert-Humblet expansion into so-called *radioactive states* [44–48]—equivalent to Eq. (2.16) in Sec. IX.2.c. of Ref. [2]—where we have modified the notation for greater consistency ($\mathcal{E}_j$ corresponds to H_λ of Ref. [2] and $\boldsymbol{r}_j$ corresponds to $\boldsymbol{\omega}_\lambda$) since there are more complex poles $\mathcal{E}_j$ than real energy levels E_λ. The Siegert-Humblet parameters are then the poles $\{\mathcal{E}_j\}$ and residue widths $\{\boldsymbol{r}_j\}$ of this complex resonance expansion of the Kapur-Peierls operator $\boldsymbol{R}_L$.

The Gohberg-Sigal theory [49] provides a method for calculating these poles and residues by solving the following generalized eigenvalue problem—which we call the *radioactive problem*:

$$\boldsymbol{R}_L^{-1}(E)|_{E=\mathcal{E}_j} \boldsymbol{q}_j = \boldsymbol{0}, \tag{11}$$

that is, finding the poles $\{\mathcal{E}_j\}$ of the Kapur-Peierls operator, $\boldsymbol{R}_L$, and their associated eigenvectors $\{\boldsymbol{q}_j\}$. The poles are complex and usually decomposed as

$$\mathcal{E}_j \triangleq E_j - i\frac{\Gamma_j}{2}. \tag{12}$$

It can be shown (cf. Sec. IX.2.d, pp. 297–298, in Ref. [2], and Sec. 9.2, Eq. (9.11), in Ref. [28]) that fundamental physical properties (conservation of probability, causality, and time reversal) ensure that the poles reside either on the positive semiaxis of purely imaginary $k_c \in i\mathbb{R}_+$—corresponding to bound states for real subthreshold energies, i.e., $E_j < E_{T_c}$ and $\Gamma_j = 0$—or that all the other poles are on the lower-half k_c plane, with $\Gamma_j > 0$, corresponding to "resonance" or "radioactively decaying" states. All poles enjoy the specular symmetry property: If $k_c \in \mathbb{C}$ is a pole of the Kapur-Peierls operator, then $-k_c^*$ is too.

Let $M_j = \dim(\mathrm{Ker}(\boldsymbol{R}_L^{-1}(\mathcal{E}_j)))$ be the dimension of the nulls pace of the inverse of the Kapur-Peierls operator at pole value $\mathcal{E}_j$, that is, M_j is the geometric multiplicity. We can thus write $\mathrm{Ker}(\boldsymbol{R}_L^{-1}(\mathcal{E}_j)) = \mathrm{Span}(\boldsymbol{q}_j^1, \ldots, \boldsymbol{q}_j^m, \ldots, \boldsymbol{q}_j^{M_j})$. As we discuss in Sec. IV C, it is physically reasonable to assume that the geometric and algebraic multiplicities are equal (semisimplicity condition), which entails a Laurent development of order 1 for the poles—i.e., no higher powers of $\frac{1}{E-\mathcal{E}_j}$ in expansion (9). Since $\boldsymbol{R}_L$ is complex symmetric, if we assume we can find nonquasinull eigenvectors solutions to (11)—that is, $\forall\ (j,m)\ ,\ \ \boldsymbol{q}_j^{m\mathsf{T}} \boldsymbol{q}_j^m \neq 0$ so it is nondefective [50–56]—then Gohberg-Sigal theory can be adapted to the case of complex-symmetric matrices to normalize the rank-M_j residues of $\boldsymbol{R}_L$ matrix as

$$\sum_{m=1}^{M_j} \boldsymbol{r}_j^m \boldsymbol{r}_j^{m\mathsf{T}} = \sum_{m=1}^{M_j} \frac{\boldsymbol{q}_j^m \boldsymbol{q}_j^{m\mathsf{T}}}{\boldsymbol{q}_j^{m\mathsf{T}} \left(\frac{\partial \boldsymbol{R}_L^{-1}}{\partial E}\big|_{E=\mathcal{E}_j}\right) \boldsymbol{q}_j^m}. \tag{13}$$

The residue widths $\{\boldsymbol{r}_j^m\}$, here called *radioactive widths*, can thus directly be expressed as

$$\boldsymbol{r}_j^m = \frac{\boldsymbol{q}_j^m}{\sqrt{\boldsymbol{q}_j^{m\mathsf{T}} \left(\frac{\partial \boldsymbol{R}_L^{-1}}{\partial E}\big|_{E=\mathcal{E}_j}\right) \boldsymbol{q}_j^m}}, \tag{14}$$

where $\frac{\partial \boldsymbol{R}_L^{-1}}{\partial E}|_{E=\mathcal{E}_j}$ can readily be calculated by means of the following property,

$$\left.\frac{\partial \boldsymbol{R}_L^{-1}}{\partial E}\right|_{E=\mathcal{E}_j} = \frac{\partial \boldsymbol{R}^{-1}}{\partial E}(\mathcal{E}_j) - \frac{\partial \boldsymbol{L}}{\partial E}(\mathcal{E}_j), \tag{15}$$

where the R-matrix $\boldsymbol{R}$ is invertible at the radioactive poles $\{\mathcal{E}_j\}$, with

$$\frac{\partial \boldsymbol{R}^{-1}}{\partial E}(E) = -\boldsymbol{R}^{-1} \boldsymbol{\gamma}^{\mathsf{T}} (\boldsymbol{e} - E\mathbb{I})^{-2} \boldsymbol{\gamma} \boldsymbol{R}^{-1}. \tag{16}$$

In practice, we are most often presented with nondegenerate states where $M_j = 1$, meaning the kernel is an eigenline $\mathrm{Ker}(\boldsymbol{R}_L^{-1}(\mathcal{E}_j)) = \mathrm{Span}(\boldsymbol{q}_j)$, which entails rank 1 residues normalized as

$$\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}} = \frac{\boldsymbol{q}_j \boldsymbol{q}_j^{\mathsf{T}}}{\boldsymbol{q}_j^{\mathsf{T}} \left(\frac{\partial \boldsymbol{R}_L^{-1}}{\partial E}\big|_{E=\mathcal{E}_j}\right) \boldsymbol{q}_j} \tag{17}$$

or equivalently

$$\boldsymbol{r}_j^{\mathsf{T}} \left(\left.\frac{\partial \boldsymbol{R}_L^{-1}}{\partial E}\right|_{E=\mathcal{E}_j}\right) \boldsymbol{r}_j = 1; \tag{18}$$

thus, for clarity of reading and without loss of generality, we henceforth drop the superscript "m" and summation over the multiplicity, unless it is of specific interest.

The *radioactive poles*, $\{\mathcal{E}_j\}$, and *radioactive widths*, $\{\boldsymbol{r}_j^m = [r_{j,c_1}^m, \ldots, r_{j,c}^m, \ldots, r_{j,c_{N_c}}^m]^{\mathsf{T}}\}$, are the Siegert-Humblet parameters. They are complex and locally untangle the energy dependence into an expansion sum of poles and residues (9). Additional discussion on these poles and residues can be found in Ref. [2], Secs. IX.2.c–e, pp. 297–298, or in Refs. [44–46,48].

The Kapur-Peierls matrix $\boldsymbol{R}_L$ is invariant to a change in boundary conditions B_c—cf. Eqs. (25) and (26) of Sec. II.F of Ref. [22]—this entails that the radioactive poles $\{\mathcal{E}_j\}$ and widths $\{\boldsymbol{r}_j\}$ are independent of the boundary condition B_c.

B. Level matrix $A(E)$ approach to Siegert and Humblet expansion

An alternative approach to calculating the Siegert-Humblet parameters $\{a_c, \mathcal{E}_j, r_{j,c}^m, E_{T_c}\}$ from the Wigner-Eisenbud ones $\{a_c, B_c, \gamma_{\lambda,c}, E_\lambda, E_{T_c}\}$ is through the level matrix $\boldsymbol{A}$. We search

for the poles and eigenvectors of the level matrix operator $\boldsymbol{A}$,

$$\boldsymbol{A}^{-1}(E)|_{E=\mathcal{E}_j}\boldsymbol{b_j} = \boldsymbol{0}, \tag{19}$$

from (8); this means solving for the eigenvalues $\{\mathcal{E}_j\}$ and associated eigenvectors $\{\boldsymbol{b_j}\}$ that satisfy

$$[\boldsymbol{e} - \boldsymbol{\gamma}(\boldsymbol{L}(\mathcal{E}_j) - \boldsymbol{B})\boldsymbol{\gamma}^\mathsf{T}]\boldsymbol{b_j} = \mathcal{E}_j\boldsymbol{b_j}. \tag{20}$$

This problem is analogous to the alternative parametrization of R-matrix theory, but with replacing the shift factor $\boldsymbol{S}$ with the outgoing-wave reduced logarithmic derivative $\boldsymbol{L}$ (cf. Ref. [22]).

Again, the same hypotheses as for the Kapur-Peierls operator $\boldsymbol{R}_L$ in Sec. II A allow us to adapt the Gohberg-Sigal theory to the case of complex-symmetric operators to yield the following local Mittag-Leffler expansion of the level matrix (with normalized residues):

$$\boldsymbol{A}(E) \underset{\mathcal{W}(E)}{=} \sum_{j\geqslant 1} \frac{\sum_{m=1}^{M_j} \boldsymbol{a_j^m}\boldsymbol{a_j^m}^\mathsf{T}}{E - \mathcal{E}_j} + \mathbf{Hol}_{\boldsymbol{A}}(E). \tag{21}$$

In the most frequent case of nondegenerate eigenvalues to (19), this yields rank-1 residues as

$$\boldsymbol{A}(E) \underset{\mathcal{W}(E)}{=} \sum_{j\geqslant 1} \frac{\boldsymbol{a_j}\boldsymbol{a_j}^\mathsf{T}}{E - \mathcal{E}_j} + \mathbf{Hol}_{\boldsymbol{A}}(E). \tag{22}$$

Again, under nonquasinull eigenvectors assumption $\boldsymbol{b_j^m}^\mathsf{T}\boldsymbol{b_j^m} \neq 0$, Gohberg-Sigal theory ensures the residues are normalized as

$$\boldsymbol{a_j^m}\boldsymbol{a_j^m}^\mathsf{T} = \frac{\boldsymbol{b_j^m}\boldsymbol{b_j^m}^\mathsf{T}}{\boldsymbol{b_j^m}^\mathsf{T}\left(\frac{\partial \boldsymbol{A}^{-1}}{\partial E}\big|_{E=\mathcal{E}_j}\right)\boldsymbol{b_j^m}}, \tag{23}$$

which is readily calculable from

$$\frac{\partial \boldsymbol{A}^{-1}}{\partial E}(\mathcal{E}_j) = -\mathbb{I} - \boldsymbol{\gamma}\frac{\partial \boldsymbol{L}}{\partial E}(\mathcal{E}_j)\boldsymbol{\gamma}^\mathsf{T}. \tag{24}$$

Plugging (21) into (4) and invoking the unicity of the complex residues imply the radioactive widths (14) can be obtained as

$$\boldsymbol{r_j^m} = \boldsymbol{\gamma}^\mathsf{T}\boldsymbol{a_j^m}. \tag{25}$$

This is an interesting and novel way to define the Siegert-Humblet parameters, which is similar to the alternative parameters definition of Ref. [22]. From this perspective, the alternative parameters appear as a special case that leave the Siegert-Humblet level-matrix parameters invariant to boundary condition B_c. Indeed, one could search for the Siegert-Humblet expansion of the alternative parametrization of R-matrix theory, by simply proceeding as in Eq. (34) in Sec. III.A of Ref. [22], but replacing the level matrix $\boldsymbol{A}$ with the alternative level matrix $\widetilde{\boldsymbol{A}}$ (defined in Eqs. (30) and (33) in Sec. III.A of Ref. [22]):

$$\widetilde{\boldsymbol{A}}^{-1}(E)|_{E=\mathcal{E}_j}\widetilde{\boldsymbol{b_j}} = \boldsymbol{0}. \tag{26}$$

The exact same Gohberg-Sigal procedure can then be applied to the Mittag-Leffler expansion of the alternative level matrix $\widetilde{\boldsymbol{A}}$, in the vicinity $\mathcal{W}(E)$ of $E \in \mathbb{C}$ away from branch points $\{E_{T_c}\}$,

$$\widetilde{\boldsymbol{A}}(E) \underset{\mathcal{W}(E)}{=} \sum_{j\geqslant 1} \frac{\sum_{m=1}^{M_j} \widetilde{\boldsymbol{a_j^m}}\widetilde{\boldsymbol{a_j^m}}^\mathsf{T}}{E - \mathcal{E}_j} + \mathbf{Hol}_{\widetilde{\boldsymbol{A}}}(E), \tag{27}$$

yielding the normalized residue widths,

$$\widetilde{\boldsymbol{a_j^m}}\widetilde{\boldsymbol{a_j^m}}^\mathsf{T} = \frac{\widetilde{\boldsymbol{b_j^m}}\widetilde{\boldsymbol{b_j^m}}^\mathsf{T}}{\widetilde{\boldsymbol{b_j^m}}^\mathsf{T}\left(\frac{\partial \widetilde{\boldsymbol{A}}^{-1}}{\partial E}\big|_{E=\mathcal{E}_j}\right)\widetilde{\boldsymbol{b_j^m}}}, \tag{28}$$

where (24) can be combined to Eq. (33) of Ref. [22],

$$\boldsymbol{\gamma}^\mathsf{T}\boldsymbol{A}\boldsymbol{\gamma} = \widetilde{\boldsymbol{\gamma}}^\mathsf{T}\widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{\gamma}},$$

to calculate the energy derivative. Then, plugging (28) into the same Eq. (33) of Ref. [22], we obtain the relation between the alternative R-matrix parameters and the Siegert-Humblet radioactive state parameters:

$$\boldsymbol{r_j^m} = \widetilde{\boldsymbol{\gamma}}^\mathsf{T}\widetilde{\boldsymbol{a_j^m}}. \tag{29}$$

This relation (29) is especially enlightening when compared to (25) from the viewpoint of invariance to boundary condition B_c. Indeed, we explained that the Siegert-Humblet parameters $\{\mathcal{E}_j, \boldsymbol{r_j^m}\}$ are invariant with a change of boundary condition $B_c \to B_c'$. This is, however, not true of the level matrix residue widths $\{\boldsymbol{a_j^m}\}$ from (23). Thus, we can formally write this invariance by differentiating (25) with respect to B_c and noting that $\frac{\partial \boldsymbol{r_j^m}}{\partial \boldsymbol{B}} = \boldsymbol{0}$, yielding

$$\boldsymbol{0} = \frac{\partial \boldsymbol{\gamma}^\mathsf{T}}{\partial \boldsymbol{B}}\boldsymbol{a_j^m} + \boldsymbol{\gamma}^\mathsf{T}\frac{\partial \boldsymbol{a_j^m}}{\partial \boldsymbol{B}}. \tag{30}$$

This new relation links the variation of the Wigner-Eisenbud resonance widths $\gamma_{\lambda,c}$ at level values E_λ (resonance energies) under a change of boundary conditions $B_{c'}$, to the variation of the level matrix residue widths $a_{j,c}^m$ at pole values $\mathcal{E}_j$ under change of boundary condition $B_{c'}$. Since transformations (26) and (27) of Sec. II.F in Ref. [22] detail how to perform $\frac{\partial \boldsymbol{\gamma}^\mathsf{T}}{\partial \boldsymbol{B}}$, Eq. (30) could be used to update $\boldsymbol{a_j^m}$ under a change $B_c \to B_{c'}$.

Another telling insight from relation (30) is when we apply it to the relation between the alternative parameters and the Siegert-Humblet radioactive widths (29). Since the alternative parameters $\widetilde{\boldsymbol{\gamma}}$ are invariant to B_c (that is their main purpose), the same differentiation as in Eq. (30) now yields zero derivatives,

$$\boldsymbol{0} = \widetilde{\boldsymbol{\gamma}}^\mathsf{T}\frac{\partial \widetilde{\boldsymbol{a_j^m}}}{\partial \boldsymbol{B}}. \tag{31}$$

This is obvious from the fact that the alternative level matrix $\widetilde{\boldsymbol{A}}$ is invariant under change of boundary condition. Yet invariance (31) is insightful as it presents the alternative parameters $\{\widetilde{E}_i, \widetilde{\gamma}\}$ as the ones which, when transformed to Siegert-Humblet radioactive state parameters $\{\mathcal{E}_j, \boldsymbol{r_j}\}$ though (29), leave the level residue widths $\{\widetilde{\boldsymbol{a_j}}\}$ invariant to B_c.

Conversely, the Kapur-Peierls pole expansion (10) extends the alternative parametrization in that it generates boundary condition B_c independent poles $\{\mathcal{E}_j\}$ and radioactive widths $\{\boldsymbol{r_j}\}$ that explicitly invert the alternative level matrix $\widetilde{\boldsymbol{A}}$ to yield (27).

C. Siegert-Humblet radioactive pole expansion branch structure

Section II A introduced the Siegert-Humblet parametrization as the solutions of radioactive problem (11), where the $\boldsymbol{R}(E)$ matrix (5) is a function of the energy E, while $\boldsymbol{L}(\boldsymbol{\rho})$ is a function of the dimensionless wave number $\rho_c \triangleq a_c k_c(E)$. Thus, radioactive problem (11) can be solved either in energy space or in momentum space, both of which are linked by the $\rho(E)$ mapping (1). This mapping induces a multisheeted Riemann surface, which introduces branch points and sheets we now unveil in Theorem 1.

Theorem 1. SIEGERT-HUMBLET RADIOACTIVE POLE EXPANSION BRANCH STRUCTURE.

Let the radioactive poles $\{\mathcal{E}_j\}$ be the solutions of the radioactive problem (11) and $\{E_{T_c}\}$ denote the threshold energies and branch points of the $\rho_c(E)$ wave-number energy mapping (1); then

(1) In the neighborhood $\mathcal{W}(E)$ of any complex energy E away from branch points $\{E_{T_c}\}$, there exists a series of complex matrices $\{\boldsymbol{c}_n\}$ such that the Mittag-Leffler expansion (10) takes the analytic form

$$\boldsymbol{R}_L(E) \underset{\mathcal{W}(E)}{=} \sum_{j\geqslant 1} \frac{\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}}}{E-\mathcal{E}_j} + \sum_{n\geqslant 0} \boldsymbol{c}_n E^n. \tag{32}$$

(2) The radioactive poles $\{\mathcal{E}_j\}$ are complex and live on the multisheeted Riemann surface of $k_c(E)$ wave-number energy mapping (1):

$$\{\mathcal{E}_j, +, +, -, \cdots, +, -\}. \tag{33}$$

(3) Let N_L be the number of solutions to the radioactive problem (11) in wave-number $\boldsymbol{\rho}$ space. For every sheet of the of the wave-number energy mapping (1), each pole of the R-matrix (resonance energy E_λ level) yields two radioactive poles, and each pole of the outgoing wave function reduced logarithmic derivative operator $L_c(\rho_c)$ (the ω_n of Mittag-Leffler expansion (7) established in Theorem 1 of Sec. II.B and documented in Tables I and II of Ref. [22]) yields another additional pole.

(4) For neutral particles, denoting $N_{E_{T_c}\neq E_{T_{c'}}}$ the number of channels with different thresholds, this entails the number N_L of radioactive poles is

$$N_L = \left(2N_\lambda + \sum_{c=1}^{N_c} \ell_c\right) \times 2^{\left(N_{E_{T_c}\neq E_{T_{c'}}}-1\right)}. \tag{34}$$

(5) For charged particles, this entails an infinite number (countable) of radioactive poles: $N_L = \infty$.

Proof. Away from the branch points $\{E_{T_c}\}$, the holomorphic part of Mittag-Leffler expansion (10) can be analytically expanded in series as (32)—we here assumed the nondegenerate case of rank-1 residues (multiplicity $M_j = 1$) though it is readily generalizable to (9).

When solving radioactive problem (11) or (20) to obtain the Siegert-Humblet poles $\{\mathcal{E}_j\}$ and residues $\{\boldsymbol{r}_j\}$, or $\{\boldsymbol{a}_j\}$, it is necessary to compute the $\boldsymbol{L}^{\boldsymbol{0}}$ matrix function $\boldsymbol{L}^{\boldsymbol{0}}(E) \triangleq \boldsymbol{L}^{\boldsymbol{0}}(\boldsymbol{\rho}(E))$ for complex energies $E \in \mathbb{C}$. As discussed in Ref. [22] (cf. Secs. II.A, II.B, III.B, and III.C of Ref. [22]), mapping (1) generates a multisheeted Riemann surface with 2^{N_c} branches (with the threshold values E_{T_c} as branch points), corresponding to the choice for each channel c, of the sign of the square root in $\boldsymbol{\rho}(E)$. This means that when searching for the poles, one has to keep track of these choices and specify for each pole $\mathcal{E}_j$ on what sheet it is found. Every pole $\mathcal{E}_j$ must thus come with the full reporting of these N_c signs, i.e., $\{\mathcal{E}_j, -, +, +, \cdots, -, +\}$ as (33).

When searching for these radioactive poles in wave-number space, the $\boldsymbol{R}_L$ Kapur-Peierls operator (4) is continued to complex wave numbers by meromorphic continuation of $\boldsymbol{L}(\boldsymbol{\rho})$, where the reduced logarithmic derivative of the outgoing wave function (6) takes the Mittag-Leffler expansion described in Eq. (13) of Theorem 1, Sec. II.B, of Ref. [22]. There are more radioactive poles $\{\mathcal{E}_j\}$ than Wigner-Eisenbud levels $\{E_\lambda\}$—as was the case for the alternative parameters (cf. Theorems 2 and 3 in Sec. III.C of Ref. [22]). For massive neutral particles, we can proceed in an analogous fashion as for the proof of Theorem 3 in Sec. III.C of Ref. [22], and apply the diagonal divisibility and capped multiplicities lemma (Lemma 3 in Sec. III.C of Ref. [22]) to the determinant of the Kapur-Peierls operator $\boldsymbol{R}_L$ in Eq. (11)—but this time in ρ_c space—and then look at the order of the resulting rational fractions in ρ_c and the number of times one must square the polynomials to unfold all $\rho_c = \mp\sqrt{\cdot}$ sheets of mapping (1). We were thus able to establish that the number N_L of poles in wave-number ρ space is $2N_\lambda + \sum_{c=1}^{N_c} \ell_c$ poles per sheet, capped by the level multiplicities (cf. Eq. (50) of Ref. [22]):

$$N_L/2^{\left(N_{E_{T_c}\neq E_{T_{c'}}}-1\right)} = N_\lambda + \sum_{\substack{L_c \text{ multiplicity} \\ \text{capped at } N_\lambda}} \ell_c, \tag{35}$$

which in practice falls back to (34) over all sheets (there are rarely fewer levels than the number of different channels that have the exact same $L_c(\rho_c)$ function), where $N_{E_{T_c}\neq E_{T_{c'}}}$ designates the number of different thresholds (including the obvious $E_{T_c} = 0$ zero threshold) and thus the number of sheets.

In the charged particles case, $L_c(\rho_c)$ has a countably infinite number of poles, which in turn induces an infinite number (countable) of solutions to the radioactive problem (11), though the discussion after the proof of Theorem 1 in Sec. II.B of Ref. [22] shows most of these poles are far-away poles, and only ℓ_c ones are within a closer range. ■

It is important to grasp the meaning of the Mittag-Leffler expansion (10)—or (21) and (27). These are local expressions: They do not hold for all complex energies $E \in \mathbb{C}$ because of the branch-point structure of the Riemann sheet. However, in the neighborhood $\mathcal{W}(E)$ of any complex energy point $E \in \mathbb{C}$ away from the branch points (thresholds $\{E_{T_c}\}$), the Mittag-Leffler expansion (10) is true, and its holomorphic part admits an analytic expansion $\mathbf{Hol}_{\boldsymbol{R}_L}(E) \triangleq \sum_{n\geqslant 0} \boldsymbol{c}_n E^n$. This has two major consequences for the Siegert-Humblet expansion. First, contrary to the alternative parameters $\{\widetilde{E}_i, \widetilde{\gamma_{i,c}}\}$ discussed in Ref. [22], the Siegert-Humblet set of radioactive

poles and widths $\{\mathcal{E}_j, r_{j,c}\}$ do not suffice to uniquely determine the energy behavior of the scattering matrix $\boldsymbol{U}(E)$: One needs to locally add the expansion coefficients $[\boldsymbol{c}_n]_{c,c'}$ of the entire part $\mathbf{Hol}_{\boldsymbol{R}_L}(E) \triangleq \sum_{n\geqslant 0} \boldsymbol{c}_n E^n$. Second, since the set of coefficients $\{\boldsymbol{c}_n\}$ is *a priori* infinite (and so is the set of poles in the Coulomb case), this means that numerically the Siegert-Humblet expansion can only be used to compute local approximations of the scattering matrix, which can nonetheless reach any target accuracy by increasing the number of $\{\mathcal{E}_j\}_{j\in[\![1,N_L]\!]}$ poles included and the order of the truncation $N_{\mathcal{W}(E)}$ in $\{\boldsymbol{c}_n\}_{n\in[\![1,N_{\mathcal{W}(E)}]\!]}$. In practice, this means that to compute the scattering matrix one needs to provide the Siegert-Humblet parameters $\{\mathcal{E}_j, r_{j,c}\}$, cut the energy domain of interest into local windows $\mathcal{W}(E)$ away from threshold branch points $\{E_{T_c}\}$, and provide a set of local coefficients $\{\boldsymbol{c}_n\}_{n\in[\![1,N_{\mathcal{W}(E)}]\!]}$ for each window.

As discussed in Ref. [22] (cf. Lemmas 1 and 2 in Sec. III.B and Theorems 2 and 3 of Sec. III.C of Ref. [22]), the definition of the shift and penetration functions for complex wave numbers is ambiguous (in particular, purely imaginary wave numbers yield negative or subthreshold energies), which in turn entail various possible alternative parameters. When solving radioactive problem (11) to find the Siegert-Humblet radioactive poles and residues $\{\mathcal{E}_j, r_{j,c}\}$—or (20) equivalently—there are no such ambiguities on the definition of $\boldsymbol{L}$: The Kapur-Peierls operator is simply analytically continued to complex wave numbers. The unicity of analytic continuation thus entails that the Siegert-Humblet parameters are uniquely defined, as long as we specify for each channel c what sheet of the Riemann surface from mapping (1) was chosen, as in Eq. (33).

The $\{\mathcal{E}_j, +, +, \cdots, +, +\}$ sheet is called the *physical sheet*, and we here call the poles on that sheet the *principal poles*. All other sheets are called *nonphysical* and the poles laying on these sheets are called *shadow poles*. Often, the principal poles are responsible for the resonant behavior, with shadow poles only contributing to background behavior, but cases have emerged where the shadow poles contribute significantly to the resonance structure, as reported in Ref. [57], and Hale there introduced a quantity called *strength* of a pole (cf. Eq. (7) in Ref. [57], and the paragraph after Eq. (2.11) in Sec. XI.2.b, p. 306, and Sec. XI.4, p. 312 in Ref. [2]) to quantify the impact a pole $\mathcal{E}_j$ will have on resonance behavior, by comparing the residue $r_{j,c}$ to the Wigner-Eisenbud widths $\gamma_{\lambda,c}$.

Result (34) is quite instructive: One can observe that the number N_L of Siegert-Humblet poles adds up to the number of levels N_λ and the number of poles of $\boldsymbol{L}$ (which is $\sum_{c=1}^{N_c} \ell_c$ for neutral massive particles and is infinite in the Coulomb case; cf. discussion after Theorem 1 in Sec. II.B of Ref. [22]). Moreover, N_L is duplicated with each new sheet of the Riemann surface from mapping (1) that is associated to a new threshold, and hence the $N_{E_{T_c}\neq E_{T_{c'}}}$. Interestingly, after comparing N_L from (34) with the number N_S of alternative analytic poles from Eq. (49) in Theorem 3 of Sec. III.C of Ref. [22]—which are in E space and must thus be doubled to obtain the number of ρ-space poles—we note that the analytic continuation of the shift factor $\boldsymbol{S}$ (cf. Lemma 2 in Sec. III.B of Ref. [22]) adds a virtual pole for each pole of $\boldsymbol{L}$ when unfolding the sheets of mapping (1), because it is a function of $\rho_c^2(E)$. This can readily be observed in the trivial case of a p wave ($\ell = 1$) channel with one resonance (one level $N_\lambda = 1$), where $S(E) = -\frac{1}{1+\rho^2(E)}$ introduces two poles at $\rho(E) = \pm i$, while $L(E) = \frac{-1+i\rho(E)+\rho^2(E)}{1-i\rho(E)}$ only counts one pole, at $\rho(E) = i$.

As for Eq. (50) of Theorem 3 in Sec. III.C of Ref. [22], one should add the precision that in the sum over the channels in Eq. (34), the multiplicity of possible $L_c(\rho_c)$ repeated over many different channels $L_c(\rho_c) = L_{c'\neq c}(\rho_{c'})$ is capped by N_λ, which in practice would only occur in the rare cases where only one or two levels occurs for many channels with same angular momenta (and, of course, total angular momenta and parity J^π).

Numerically, solving the generalized eigenvalue problems (11) or (20) falls into the well-known class of nonlinear eigenvalue problems, for which algorithms we direct the reader to Chap. 115 in *The Handbook of Linear Algebra* [58]. We will just state that instead of the Rayleigh-quotient type of methods expressed in Ref. [58], it can sometimes be computationally advantageous to first find the poles $\{\mathcal{E}_j\}$ by solving the channel determinant problem, $\det(\boldsymbol{R}_L^{-1}(E)|_{E=\mathcal{E}_j}) = 0$, or the corresponding level determinant one, $\det(\boldsymbol{A}^{-1}(E)|_{E=\mathcal{E}_j}) = 0$, and then solve the associated linear eigenvalue problem. Methods tailored to find all the roots of this problem were introduced in Ref. [59] and in Eqs. (200) and (204) of Ref. [60]. Notwithstanding, from a numerical standpoint, having the two approaches is beneficial in that solving (11) will be advantageous over solving (20) when the number of levels N_λ far exceeds the number of channels N_c and vice versa. Nonetheless, the multisheeted nature of the radioactive problem makes it harder to solve, as one must search each sheet of mapping (1) to find all the poles.

D. Xenon isotope ^{134}Xe evidence of radioactive state parameters

In our previous article [22], we observed the first evidence of shadow poles in the alternative parametrization of R-matrix theory in xenon isotope ^{134}Xe spin-parity group $J^\pi = 1/2^{(-)}$, showing how they depend on the choice of continuation to complex wave numbers. We here document in Table I the Siegert-Humblet radioactive state parameters (poles and residues of the Kapur-Peierls $\boldsymbol{R}_L$ operator) for these same p-wave resonances of ^{134}Xe spin-parity group $J^\pi = 1/2^{(-)}$. As shown in Fig. 1, both the radioactive state parameters and the R-matrix parameters yield an identical Kapur-Peierls $\boldsymbol{R}_L(E)$ operator, and therefore exactly reconstruct the scattering matrix $\boldsymbol{U}(E)$ of the nuclear interactions, as reported in Fig. 2. Note there are $N_L = 5$ radioactive poles, as predicted by (34) in Theorem 1: two for each resonance energy E_λ level and ℓ_c for each $L_c(\rho_c)$ channel. Indeed, we here have only one threshold (at zero) so that $N_{E_{T_c}\neq E_{T_{c'}}} = 1$, and there is only one channel, for which $\ell_c = 1$ (p wave). As such, we observe in Table I that for each resonance energy E_λ, there are two nearby radioactive poles, each on one sheet of the Riemann surface energy–wave-number mapping (1), and both close to (but not exactly) complex conjugates of one another. Also, the additional radioactive pole (the first in Table I) is close to the corresponding pole of the reduced logarithmic derivative of the outgoing operator $L_c(\rho_c)$: For neutral particle p waves, we have $\omega_1^{\ell=1} = -i$ (see Table I of Ref. [22]), which

TABLE I. Radioactive state parameters [Siegert-Humblet poles and residue widths of the Kapur-Peierls $\boldsymbol{R}_L(E)$ operator] of the two p-wave resonances of ^{134}Xe, spin-parity group $J^\pi = 1/2^{(-)}$, converted from ENDF/B-VIII.0 evaluation (MLBW) to multipole representation using Reich-Moore level matrix (8), that is, Definition (58) of Ref. [22].

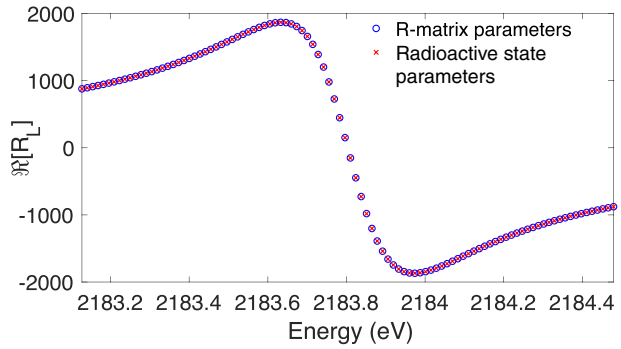
Nuclear data
$z = \sqrt{E}$ with E in (eV)
$A = 132.7600$
$\rho_0 = \frac{Aa_c\sqrt{\frac{2m_n}{\hbar}}}{A+1}$ in $(\sqrt{\text{eV}}^{-1})$, so that $\rho(z) \triangleq \rho_0 z$
with $\sqrt{\frac{2m_n}{\hbar}} = 0.002196807122623$ in units $[1/(10^{-14}\text{m}\sqrt{\text{eV}})]$
***R*-matrix parameters**
$a_c = 5.80$: channel radius (Fermis)
$E_1 = 2186.0$: 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
$B_c = -1$

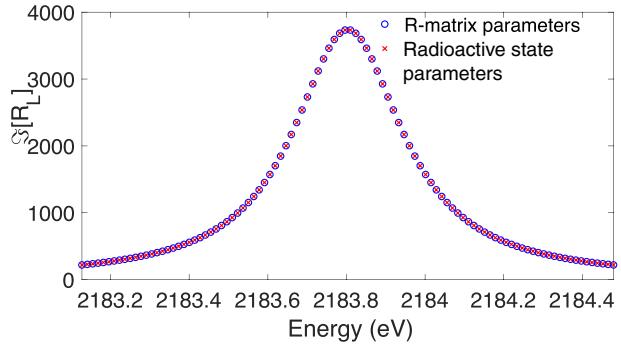
Radioactive state parameters (rounded to five digits)

Radioactive poles $\{\mathcal{E}_j, \pm\}$ from (20) (eV), sheet of (1)	Radioactive residue widths $\boldsymbol{r}_j$ from (25) $(\sqrt{\text{eV}})$	Level-matrix residue widths $\boldsymbol{a}_j$ from (22) (dimensionless)
$\left\{\begin{matrix}-6.2694\times10^{+5}\\ -i1.0238\times10^{-4}, +\end{matrix}\right\}$	$\begin{matrix}9.1193\times10^{-8}\\ -i1.4762\times10^{+0}\end{matrix}$	$\left[\begin{matrix}2.7683\times10^{-9}\\ -i4.4744\times10^{-2}\\ \hline 1.5345\times10^{-9}\\ -i2.4964\times10^{-2}\end{matrix}\right]$
$\left\{\begin{matrix}2.1838\times10^{+3}\\ +i9.0757\times10^{-2}, -\end{matrix}\right\}$	$\begin{matrix}8.6799\times10^{-4}\\ -i2.5113\times10^{+1}\end{matrix}$	$\left[\begin{matrix}4.444\times10^{-5}\\ -i9.995\times10^{-1}\\ \hline -1.7608\times10^{-5}\\ -i2.9849\times10^{-4}\end{matrix}\right]$
$\left\{\begin{matrix}2.1838\times10^{+3}\\ -i1.6868\times10^{-1}, +\end{matrix}\right\}$	$\begin{matrix}8.6814\times10^{-4}\\ +i2.5113\times10^{+1}\end{matrix}$	$\left[\begin{matrix}4.444\times10^{-5}\\ +i9.995\times10^{-1}\\ \hline -1.7597\times10^{-5}\\ +i2.9849\times10^{-4}\end{matrix}\right]$
$\left\{\begin{matrix}6.3130\times10^{+3}\\ +i1.6025\times10^{-1}, -\end{matrix}\right\}$	$\begin{matrix}2.4919\times10^{-3}\\ -i1.4085\times10^{+1}\end{matrix}$	$\left[\begin{matrix}8.5974\times10^{-5}\\ +i8.5696\times10^{-4}\\ \hline 2.3534\times10^{-5}\\ -i9.9984\times10^{-1}\end{matrix}\right]$
$\left\{\begin{matrix}6.3130\times10^{+3}\\ -i2.3822\times10^{-1}, +\end{matrix}\right\}$	$\begin{matrix}2.4916\times10^{-3}\\ +i1.4085\times10^{+1}\end{matrix}$	$\left[\begin{matrix}8.5964\times10^{-5}\\ -i8.5697\times10^{-4}\\ \hline 2.3534\times10^{-5}\\ +i9.9984\times10^{-1}\end{matrix}\right]$

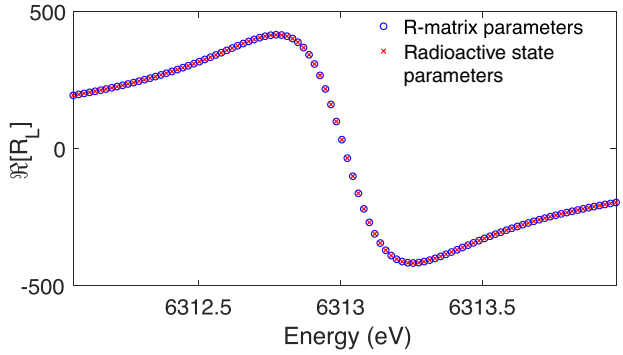
entails a radioactive pole close to $(\frac{i}{\rho_0})^2 \approx -6.0673\times10^{+5}$. Incidentally, note that if there were only one level $N_\lambda = 1$, but two channels $N_c = 2$, both with the same angular momentum (say, p waves) and the same $\rho_c(E)$ mapping, then we would need to cap the multiplicity of the number of poles induced by these identical $L_c(\rho_c)$ to $N_\lambda = 1$, according to Eq. (35). This is rare in practice.

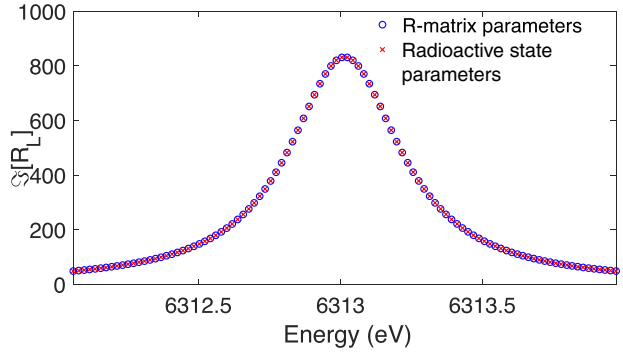
The exact reconstruction of the scattering matrix $\boldsymbol{U}(E)$ shown in Fig. 2 is made possible because ^{134}Xe spin-parity group $J^\pi = 1/2^{(-)}$ has only a neutron channel with zero threshold ($E_{T_c} = 0$). In the particular case of neutral particles with zero threshold, the outgoing wave-function reduced logarithmic derivative operator $\boldsymbol{L}(\boldsymbol{\rho})$ is a rational function in $\sqrt{E}$: This can be seen from Mittag-Leffler expansion (7) with a finite amount of poles $\{\omega_n\}$ (reported in Theorem 1 of Sec. II.B and Table II of Ref. [22]). Therefore, the transformation $z \triangleq \sqrt{E}$ unfolds the Riemann surface of mapping (1): Searching for solutions to the radioactive problem (11)





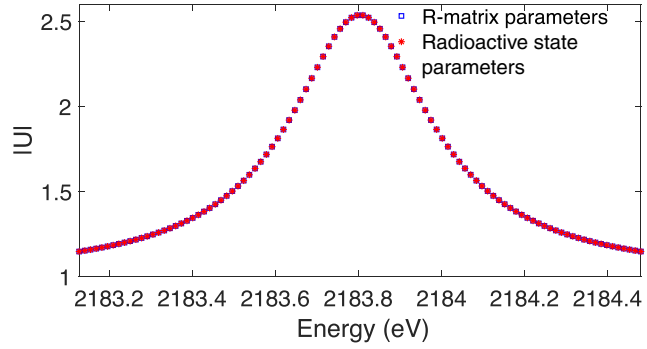
(a) First p-wave resonance.

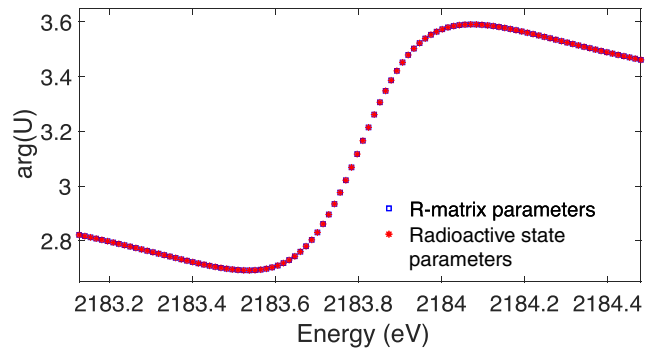




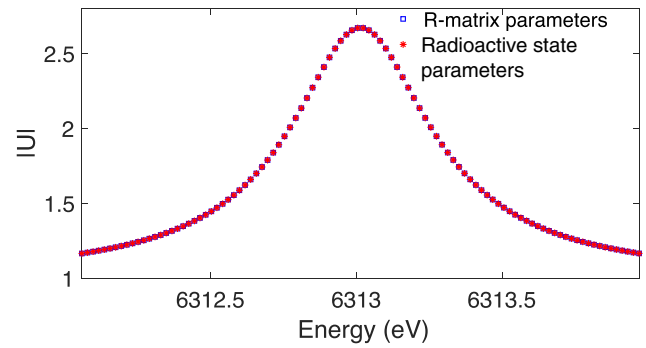
(b) Second p-wave resonance.

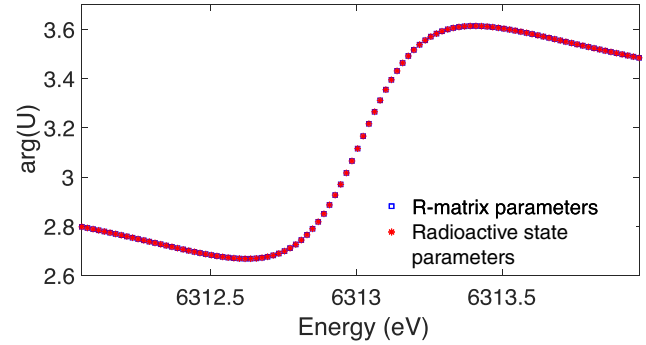
FIG. 1. Kapur-Peierls $\boldsymbol{R}_L(E)$ operator (4) of ^{134}Xe two p-wave resonances in spin-parity group $J^\pi = 1/2^{(-)}$. Dimensionless $\boldsymbol{R}_L(E)$ is computed using radioactive state parameters from Table I in expression (40) or using the R-matrix parameters from Table I in Reich-Moore level matrix (8)—that is, definition (58) of Ref. [22]—yielding identical real and imaginary parts.





(a) First p-wave resonance.





(b) Second p-wave resonance.

FIG. 2. Scattering matrix $\boldsymbol{U}(E)$ of ^{134}Xe two p-wave resonances in spin-parity group $J^\pi = 1/2^{(-)}$, from Eq. (2). Dimensionless $\boldsymbol{U}(E)$ is computed using outgoing waves $\boldsymbol{O}(E)$ from Table I of Ref. [22] and conjugacy relations (71), combined with radioactive state parameters from Table I in expression (40), or R-matrix parameters from Table I in Reich-Moore level-matrix (8)—that is, definition (58) of Ref. [22]—yielding identical moduli and arguments.

in z space is equivalent to searching on both sheets of the $\pm\sqrt{E}$ Riemann surface from mapping (1). Moreover, a study of the numerator and denominator of the inverse level matrix $\boldsymbol{A}^{-1}(z)$ from (8) then shows that the level matrix $\boldsymbol{A}(z)$ is rational function of degree -2 in z space, with N_L poles from (34) with only one sheet (no other thresholds than zero), so that its Mittag-Leffler expansion (22) is actually a partial fraction decomposition in simple z poles, without constant or holomorphic parts (cf. Sec. II.F of Ref. [36] for more in depth discussion of this process):

$$\boldsymbol{A}(E) = \sum_{j=1}^{N_L} \frac{\frac{\boldsymbol{a}_j \boldsymbol{a}_j^{\mathsf{T}}}{2\sqrt{\mathcal{E}_j}}}{\sqrt{E} - \sqrt{\mathcal{E}_j}}. \tag{36}$$

Note that the nullity of the constant term entails the following remarkable property:

$$\sum_{j=1}^{N_L} \frac{\boldsymbol{a}_j \boldsymbol{a}_j^{\mathsf{T}}}{2\sqrt{\mathcal{E}_j}} = \boldsymbol{0}. \tag{37}$$

Since from (25) we have $\boldsymbol{r_j} = \boldsymbol{\gamma}^{\mathsf{T}} \boldsymbol{a_j}$ (assuming nondegenerate states), the latter properties on the level matrix can be transcribed into the following exact pole expansion for the Kapur-Peierls operator (4):

$$\boldsymbol{R}_L(E) = \sum_{j=1}^{N_L} \frac{\frac{\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}}}{2\sqrt{\mathcal{E}_j}}}{\sqrt{E} - \sqrt{\mathcal{E}_j}}, \tag{38}$$

which is equivalent to Eq. (106) of Ref. [36], and the null constant relations (37) entails the remarkable property on the radioactive state parameters (cf. Eq. (108) of Ref. [36]):

$$\sum_{j=1}^{N_L} \frac{\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}}}{2\sqrt{\mathcal{E}_j}} = \boldsymbol{0}. \tag{39}$$

By setting a choice of sheet in $z = \pm\sqrt{E}$, the latter equations can be written as

$$\boldsymbol{R}_L(E) = \sum_{j=1}^{N_L} \frac{\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}}}{E - \mathcal{E}_j} + \underbrace{\sum_{j=1}^{N_L} \frac{\frac{\boldsymbol{r}_j \boldsymbol{r}_j^{\mathsf{T}}}{2\sqrt{\mathcal{E}_j}}}{\sqrt{E} + \sqrt{\mathcal{E}_j}}}_{\mathbf{Hol}_{\boldsymbol{R}_L}(E)}, \tag{40}$$

where $-\sqrt{\mathcal{E}_j}$ is not a pole, and therefore the second term is the exact holomorphic part $\mathbf{Hol}_{\boldsymbol{R}_L}(E)$ from (10).

E. Comparing radioactive, traditional, and alternative *R*-matrix parameters

This case of ^{134}Xe shows the general merits of the radioactive state parameters: In contrast with the R-matrix resonance parameters, the radioactive poles $\mathcal{E}_j$ are independent of both the arbitrary boundary parameter B_c and the channel radius a_c, while the radioactive widths $\boldsymbol{r_j}$ are independent of the boundary parameters B_c and depend on the channel radius in a systematic way (provided by Theorem 2 below). Moreover, in this specific neutral particles with zero-threshold case, the Kapur-Peierls $\boldsymbol{R}_L(E)$ operator pole expansions (38) and (40) are exact (cf. Fig. 1) and therefore can fully reconstruct the R-matrix model scattering matrix, as can be seen in Fig. 2.

Nonetheless, this example also shows the limitations of the radioactive state parameters pole expansion approach (32) of Theorem 1. Just as the alternative parameters of Brune in Ref. [22], the radioactive state parameters entangle the energy dimension with the wave-number one, meaning one now has to specify with each radioactive pole $\mathcal{E}_j$ its sheet (33) on the Riemann surface of mapping (1), for each threshold branch, as specified in Theorem 1. In contrast, though they depend on the arbitrary boundary parameters B_c and channel radii a_c, the traditional Wigner-Eisenbud R-matrix parameters have the truly remarkable (and seldom appreciated) property of deentangling the energy dimension from the wave-number one. The Wigner-Eisenbud resonance parameters are real and well defined in energy space, without any need to map to the wave number and therefore specify where the resonance energies E_λ dwell on the multisheeted Riemann surface of mapping (1).

Another significant limitation of the radioactive state parameters is that they are in general incomplete, meaning that the knowledge of the radioactive poles and residues is not sufficient to fully parametrize the $\boldsymbol{R}_L(E)$ Kapur-Peierls operator: One also needs to parametrize the holomorphic part $\mathbf{Hol}_{\boldsymbol{R}_L}(E)$ in Mittag-Leffler expansion (32). In the general case of charged particles or thresholds, there is no simple way of parametrizing this holomorphic part [though it is known exactly for zero-threshold neutral particles, as Eq. (40) specifies]. Moreover, even if the holomorphic part were known, in the general case of charged particles and thresholds there is an infinite number of radioactive poles ($N_L = \infty$), all of which are necessary to exactly reconstruct the scattering matrix. This means the radioactive state parameters alone are not very well suited for evaluations in standard nuclear data libraries. Nonetheless, the radioactive poles have recently been used to constitute an alternative nuclear data library—the *windowed multipole library*—with the goal of achieving significant computational performance gains in nuclear simulations, as we explain in our followup article [36]: The final in the xenon trilogy on pole parametrizations of R-matrix theory [22,36].

For comparison, the alternative parameters proposed by Brune in Ref. [20] combine some merits and drawbacks of both the radioactive and the traditional (Wigner-Eisenbud) parameters. Like the radioactive state parameters, the alternative parameters are independent of the arbitrary boundary condition B_c, though they still depend on arbitrary channel radii a_c. Like the Wigner-Eisenbud resonance parameters, the alternative parameters are always complete: With the knowledge of N_λ alternative poles, one can fully reconstruct the scattering matrix (cf. Theorem 4 of Ref. [22]). On the other hand, unlike the Wigner-Eisenbud resonance parameters, the alternative parameters entangle the energy dimension with the wave-number one: As for the radioactive poles, one must specify on which sheet of the Riemann surface (1) are the alternative poles (cf. Theorems 2 of Ref. [22]). However, proper analytic continuation will unfold the sheets of Riemann surface (1) and thus render such specification useless, as we show in Theorem 3 of Ref. [22]—this is another strong argument in favor of analytic continuation of R-matrix operators, in particular the shift $S_c(\rho_c)$ and penetration $P_c(\rho_c)$ functions

(contrarily to "force closure" legacy of Lane and Thomas). Moreover, in practice this is not as much of a limitation, as we showed in Theorem 4 of Ref. [22] that we can always choose the first N_λ resonant alternative poles of the physical sheet $\{E, +\}$. Nonetheless, all Reich-Moore and subthreshold alternative parameters still change depending on whether the shift $S_c(E)$ and penetration $P_c(E)$ functions are analytically continued (Theorem 3 of Ref. [22]) or "force closed" as defined by Lane and Thomas (Theorem 2 of Ref. [22]): We here argue that the physically and mathematically correct way is to perform analytic continuation of the shift $S_c(\rho_c)$ and penetration $P_c(\rho_c)$ functions, and provide many more arguments for this in Sec. IV.

Note that a commonly alleged advantage of the alternative poles $\widetilde{E}_\lambda$ is that they correspond to the peak of the resonances—actually of the Kapur-Peierls operator $\boldsymbol{R}_L(E)$ since the cross section has an additional $\frac{1}{|k_c(E)|^2}$ modulating term (see Ref. [36] for more discussion on this). Though this is true in the case of full R-matrix equations (where the resonance energies are real) for resonant poles above threshold (not the shadow poles discovered in Ref. [22]), this ceases to be true for channel-eliminated Reich-Moore evaluations (where the resonance energies are in effect complex $E_\lambda - \mathrm{i}\frac{\Gamma_{\lambda,\gamma}}{2}$ as explained in Sec. II.A.4 of Ref. [36]). Indeed, the alternative poles $\widetilde{E}_\lambda$ are then complex (cf. Sec. IV.A of Ref. [22]), and neither analytic continuation nor Lane and Thomas force closure will entail their real parts exactly correspond to the Kapur-Peierls operator $\boldsymbol{R}_L(E)$ resonance peaks. The exact peaks of the $\boldsymbol{R}_L(E)$ resonances are actually the real parts of the radioactive poles $\mathrm{Re}[\mathcal{E}_j]$, and the widths are the imaginary parts $\mathrm{Im}[\mathcal{E}_j]$, which we here document in Table I and show in Fig. 1 for the two p-wave resonances of ^{134}Xe spin-parity group $J^\pi = 1/2^{(-)}$. In practice, though, the real part of the alternative poles $\mathrm{Re}[\widetilde{E}_\lambda]$ are close (but not identical) to the real part of the radioactive poles $\mathrm{Re}[\mathcal{E}_j]$ (one needs to go to more digits to see the discrepancy between values of Table VI in Ref. [22] to our Table I here), and as such are much closer to the peak of the resonances than are the Wigner-Eisenbud resonance energies E_λ.

Another important characteristic of the radioactive state parameters is that they are the bridge between the R-matrix theory parametrizations of nuclear reactions, and the scattering matrix pole expansions of Humblet and Rosenfeld, as we now explain in Sec. II F.

F. Radioactive state parameters link R-matrix theory to the scattering matrix pole expansions

So far, we have started from the R-matrix Wigner-Eisenbud parameters $\{E_\lambda, \gamma_{\lambda,c}\}$ to construct the poles and residues of the Kapur-Peierls operator $\boldsymbol{R}_L$, through (11) and (14). We here show that these Siegert-Humblet radioactive state parameters are the link between R-matrix theory (cf. Refs. [2,17,18]) and the scattering matrix pole expansions of Humblet-Rosenfeld and others (cf. Refs. [23–25,28–35]).

Indeed, plugging in the Kapur-Peierls $\boldsymbol{R}_L$ operator expansion (10) into the expression of the scattering matrix (2) then yields the Mittag-Leffler expansion of the scattering matrix:

$$\boldsymbol{U}(E) \underset{\mathcal{W}(E)}{=} \boldsymbol{w} \sum_{j\geqslant 1} \frac{\boldsymbol{u}_j \boldsymbol{u}_j^\intercal}{E - \mathcal{E}_j} + \mathbf{Hol}_U(E), \tag{41}$$

where $\boldsymbol{w} \triangleq 2\mathrm{i}\mathbb{I}$ is the Wronskian (3), and the scattering residue widths $\boldsymbol{u}_j$ are defined as

$$\boldsymbol{u}_j \triangleq [\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}]_{E=\mathcal{E}_j}\boldsymbol{r}_j. \tag{42}$$

In writing (41), we have used the fact that all the resonances of the scattering matrix $\boldsymbol{U}(E)$ come from the Kapur-Peierls radioactive poles $\{\mathcal{E}_j\}$—indeed, we demonstrate in Theorem 3, Sec. IV D, that the poles $\{\omega_n\}$ of the outgoing wave function $\boldsymbol{O}(E)$ cancel out in Eq. (2) and are thus not present in the scattering matrix. Cauchy's residues theorem then allows us to evaluate the residues at the pole value to obtain Eq. (42). As for (10), if a resonance were to be degenerate with multiplicity M_j, the residues would no longer be rank 1, but instead the scattering matrix residue associated to pole $\mathcal{E}_j$ would be $\sum_{m=1}^{M_j} \boldsymbol{u}_j^m \boldsymbol{u}_j^{m\intercal}$, with $\boldsymbol{u}_j^m \triangleq [\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}]_{E=\mathcal{E}_j}\boldsymbol{r}_j^m$.

Expression (41) exhibits the advantage that the energy dependence of the scattering matrix $\boldsymbol{U}(E)$ is untangled in a simple sum. All the resonance behavior stems from the complex poles and residue widths $\{\mathcal{E}_j, u_{j,c}\}$, which yield the familiar Breit-Wigner profiles (Cauchy-Lorentz distributions) for the cross section. Conversely, all the threshold behavior and the background are described by the holomorphic part $\mathbf{Hol}_U(E)$, which can be expanded in various forms, for instance, analytically (43).

This establishes the important bridge between the R-matrix parametrizations and the Humblet-Rosenfeld expansions of the scattering matrix. More precisely, Mittag-Leffler expansion (41) is identical to the Humblet-Rosenfeld expansions (10.22a) and (10.22b) in Ref. [28] for the neutral particle case and (5.4a) and (5.4b) in Ref. [31] for the Coulomb case. We thus here directly connect the R-matrix parameters with the Humblet-Rosenfeld resonances, parametrized by their partial widths and real and imaginary poles, as described in Ref. [30]. In particular, the poles $\{\mathcal{E}_j\}$ from (12), found by solving (11), are exactly the ones defined by Eqs. (9.5) and (9.8) in Ref. [28]. The scattering residue widths $\{u_{j,c}\}$, calculated from (42), then correspond to the Humblet-Rosenfeld complex residues (10.12) in Ref. [28], from which they build their quantities $\{G_{c,n}\}$ appearing in expansions (10.22a) and (10.22b) in Ref. [28] and (5.4a) and (5.4b) in Ref. [31]. Finally, the holomorphic part $\mathbf{Hol}_U(E)$ corresponds to the regular function $Q_{c,c'}(E)$ defined between (10.14a) and (10.14b) in Ref. [28].

Just as Humblet and Rosenfeld did with $Q_{c,c'}(E)$ in Sec. 10.2 of Ref. [28] and Sec. 4 of Ref. [31], we do not give here an explicit way of calculating this holomorphic contribution $\mathbf{Hol}_U(E)$ other than stating that it is possible to expand it in various ways. Far from a threshold, an analytic series in energy space E can stand:

$$\mathbf{Hol}_U(E) \underset{\mathcal{W}(E)}{=} \sum_{n\geqslant 0} \boldsymbol{s}_n E^n. \tag{43}$$

In the immediate vicinity of a threshold, the asymptotic threshold behavior will prevail (for massive particles, $U_{c,c'} \sim k_c^{\ell_c+1} k_{c'}^{\ell_{c'}}$, cf. Eq. (10.5) in Ref. [28] and Ref. [61]), yielding an expansion in wave-number space of the form

$$\mathbf{Hol}_U(E) \underset{\mathcal{W}(E_{T_c})}{=} \sum_{n\geqslant 0} \boldsymbol{s}_n k_c^n(E). \tag{44}$$

Though there is no explicit way of linking these expansions (44) or (43) to the R-matrix Wigner-Eisenbud parameters $\{E_\lambda, \gamma_{\lambda,c}\}$, this means that the same approach as that discussed in the paragraph following Theorem 1 can be taken: One can provide a local set of coefficients $\{\boldsymbol{s}_n\}_{\mathcal{W}(E)}$ to expand the holomorphic part of the scattering matrix $\mathbf{Hol}_U(E)$, and then calculate the scattering matrix from the Mittag-Leffler expansion (41). This is at the core of the windowed multipole representation of R-matrix cross sections established in Ref. [36].

An important question is that of the radius of convergence of the Mittag-Leffler expansion (41): In other terms, how big can the vicinity $\mathcal{W}(E)$ be? Humblet and Rosenfeld analyze this problem in Sec. 1.4 of Ref. [28] and perform the Mittag-Leffler expansion (1.50). In the first paragraph on p. 538, they state that Humblet demonstrated in his Ph.D. thesis that the Mittag-Leffler series will converge for $M \geqslant 1$ for $U(k)$, though this does not investigate the multichannel case and thus the multisheeted nature of the Riemann surface stemming from mapping (1). They assume at the beginning of Sec. 10.2 that this property stands in the multichannel case and yet continue their discussion with a choice of $M = 0$ that would leave the residues diverging according to their expansion (1.50). This is one reason why we chose in this article to start from a local Mittag-Leffler expansion and then search for its domain of convergence. General mathematical scattering theory shows that the Mittag-Leffler expansion holds at least on the whole physical sheet (cf. Theorem 0.2 on p. 139 of Ref. [24]). Moreover, in Ref. [62], Eden proves that between the threshold values the scattering matrix elements are analytic functions of the energies and momenta of the incident particles', though does not specify in which form the Mittag-Leffler expansion will converge separately on each sheet. In practice, this requirement is not needed since it is often computationally more advantageous to break down an energy region between two consecutive thresholds $[E_{T_c}, E_{T_{c+1}}]$ into smaller vicinities (a compression method for efficient computation used in the windowed multipole library [36]).

As we see, by performing the Mittag-Leffler expansion (41), we have traded a finite set of real, unwound, Wigner-Eisenbud parameters $\{E_\lambda, \gamma_{\lambda,c}\}$ that completely parametrize the energy dependence of the scattering matrix through (2), with an infinite set of complex Siegert-Humblet radioactive state parameters $\{\mathcal{E}_j, r_{j,c}\}$ plus some local coefficients $\{\boldsymbol{s}_n\}_{\mathcal{W}(E)}$ for the holomorphic part, all intricately intertwined through radioactive problem (11), which makes them dwell on a submanifold of the multisheeted Riemann surface of mapping (1). This additional complexity of the Siegert-Humblet parameters comes at the gain of a simple parametrization of the energy dependence for the scattering matrix: the pole and residue expansion (41). For computational purposes, this may sometimes be a trade-off worth doing: This is the basis for the windowed multipole representation of R-matrix cross sections [36].

III. RADIOACTIVE STATE PARAMETERS INVARIANCE TO CHANNEL RADII

Section II provided new insights into the link between the Humblet-Rosenfeld scattering matrix pole expansions and both the Wigner-Eisenbud and Siegert-Humblet parametrizations of R-matrix theory. Concerning invariance to arbitrary parameters, we saw that the Siegert-Humblet parameters are invariant under change of boundary condition B_c, but not under change of channel radius a_c—this is also true for the alternative parameters discussed in Ref. [22]. This section is dedicated to invariance properties of the Siegert-Humblet radioactive state parameters to a change in channel radius a_c. This problem is less studied than that of the invariance to the boundary conditions B_c. To the best of our knowledge, the only previous results on this topic are the partial differential equations on the Wigner-Eisenbud $\{E_\lambda, \gamma_{\lambda,c}\}$ parameters Teichmann derived in his Ph.D. thesis (cf. Eqs. (2.29) and (2.31) in Sec. III.2, p. 27, of Ref. [63]), a recent study of the limit case $a_c \to 0$ in Ref. [64], as well as the general results of the variations of the R matrix to any arbitrary parameter by Mockel and Perez (cf. Eqs. (71) and (75) [65]). We here focus on the Siegert-Humblet parameters $\{\mathcal{E}_j, r_{j,c}\}$. Our main result of this section resides in Theorem 2, which establishes a way of converting the Siegert-Humblet radioactive state parameters under a change of channel radius a_c.

Theorem 2. RADIOACTIVE STATE PARAMETERS TRANSFORMATION UNDER CHANGE OF CHANNEL RADIUS a_c.

Let the radioactive poles $\{\mathcal{E}_j\}$ be the solutions of the radioactive problem (11). Under a change of channel radius $a_c^{(0)} \to a_c$ (or infinitesimal $\frac{\partial\cdot}{\partial a_c}$) the following hold:

(1) The Kapur-Peierls operator $\boldsymbol{R}_L$, defined in Eq. (4), is subject to the following partial differential equations: for the diagonal elements,

$$a_c \frac{\partial R_{Lcc}}{\partial a_c} + (1 - 2L_c) R_{Lcc} - 1 = 0, \tag{45}$$

and for off-diagonal ones,

$$a_c \frac{\partial R_{Lcc'}}{\partial a_c} + \left(\frac{1}{2} - L_c\right) R_{Lcc'} = 0. \tag{46}$$

(2) The radioactive poles $\{\mathcal{E}_j\}$ are invariant:

$$\frac{\partial \mathcal{E}_j}{\partial a_c} = 0. \tag{47}$$

(3) The radioactive widths $\{r_{j,c}\}$ [widths of the Kapur-Peierls $\boldsymbol{R}_L$ operator residues (13)] are subject to the following first-order linear partial differential equation:

$$a_c \frac{\partial r_{j,c}}{\partial a_c} + \left(\frac{1}{2} - L_c\right) r_{j,c} = 0, \tag{48}$$

(4) which can be formally solved as

$$r_{j,c}(a_c) = r_{j,c}\big(a_c^{(0)}\big)\sqrt{\frac{a_c^{(0)}}{a_c}}\,\exp\left(\int_{a_c^{(0)}}^{a_c}\frac{L_c(k_c x)}{x}dx\right) \tag{49}$$

(5) and explicitly integrates to

$$\frac{r_{j,c}(a_c)}{r_{j,c}\big(a_c^{(0)}\big)} = \frac{O_c(\rho_c(a_c))}{O_c\big(\rho_c\big(a_c^{(0)}\big)\big)}\sqrt{\frac{a_c^{(0)}}{a_c}}. \tag{50}$$

(6) Moreover, letting $\{\omega_n\}$ be the roots of the outgoing wave function $\{\omega_n \mid O_c(\omega_n) = 0\}$, the latter (50) can take the following elemental product expansion:

$$\frac{r_{j,c}(a_c)}{r_{j,c}\big(a_c^{(0)}\big)} = \sqrt{\frac{a_c^{(0)}}{a_c}}\left(\frac{a_c^{(0)}}{a_c}\right)^{\ell} \mathrm{e}^{\mathrm{i}k_c(a_c - a_c^{(0)})} \times \prod_{n\geqslant 1}\left(\frac{k_c a_c - \omega_n}{k_c a_c^{(0)} - \omega_n}\right), \tag{51}$$

where there are an infinite number of such roots $\{\omega_n\}$ in the Coulomb case, while for neutral particle channel c with angular momentum ℓ, there exists exactly ℓ roots $\{\omega_n\}_{n\in[\![1,\ell]\!]}$, the exact and algebraically solvable values of which are reported, up to angular momentum $\ell = 4$, in Table II of Ref. [22].

Proof. We start by bringing forth the observation that the scattering matrix $\boldsymbol{U}$ is invariant under change of channel radius a_c; i.e., for any channel c we have

$$\frac{\partial \boldsymbol{U}}{\partial a_c} = \boldsymbol{0}. \tag{52}$$

Since Theorem 3 will show that the poles of the scattering matrix are exactly the ones of the Kapur-Peierls operator $\boldsymbol{R}_L$, which are the Siegert-Humblet poles $\{\mathcal{E}_j\}$, invariance (52) entails that the radioactive poles are invariant under change of channel radius a_c, i.e., (47).

This is not the case for the radioactive widths $\{r_{j,c}\}$. However, one can use invariance (52) to differentiate the scattering matrix $\boldsymbol{U}$ expression (2). The $\boldsymbol{L}$ operator definition (6) and $\rho_c = k_c a_c$ entail

$$\frac{\partial \rho_c^{1/2} O_c^{-1}}{\partial a_c} = \frac{1}{a_c}\rho_c^{1/2} O_c^{-1}\left[\frac{1}{2} - L_c\right]; \tag{53}$$

this enables us to establish the partial differential equations (45) and (46) on the Kapur-Peierls matrix operator $\boldsymbol{R}_L$ elements, which can be synthesized into expression

$$\boldsymbol{a}\frac{\partial \boldsymbol{R}_L}{\partial \boldsymbol{a}} + \left(\frac{1}{2}\mathbb{I} - \boldsymbol{L}\right)\boldsymbol{R}_L + \mathbb{I}\circ\left[\left(\frac{1}{2}\mathbb{I} - \boldsymbol{L}\right)\boldsymbol{R}_L - \mathbb{I}\right] = \boldsymbol{0}, \tag{54}$$

where $\circ$ designates the Hadamard matrix product, and where we used the notation

$$\left[\frac{\partial \boldsymbol{R}_L}{\partial \boldsymbol{a}}\right]_{cc'} \triangleq \frac{\partial R_{Lcc'}}{\partial a_c}. \tag{55}$$

Equivalently, inverting the Kapur-Peierls operator in differential equation (55) yields the following Riccati equation:

$$\boldsymbol{a}\frac{\partial \boldsymbol{R}_L^{-1}}{\partial \boldsymbol{a}} - \boldsymbol{R}_L^{-1}\left(\frac{1}{2}\mathbb{I} - \boldsymbol{L}\right) - \mathbb{I}\circ\left[\boldsymbol{R}_L^{-1}\left(\frac{1}{2}\mathbb{I} - \boldsymbol{L}\right) - \boldsymbol{R}_L^{-2}\right] = \boldsymbol{0}. \tag{56}$$

These first-order partial differential equations on the Kapur-Peierls operator $\boldsymbol{R}_L$ are equivalent to relations (71) and (75) Mockel and Perez established for the $\boldsymbol{R}$ matrix in Ref. [65]. They are quite inconvenient to solve in that they are channel dependent and thus give rise to equations for each cross term. Remarkably, this is not the case for the radioactive residues.

Having demonstrated the radioactive poles invariance (47), Mittag-Leffler expansion (41) entails that $\boldsymbol{u_j}$ from (42) satisfies invariance: $\frac{\partial \boldsymbol{u_j}}{\partial a_c} = \boldsymbol{0}$. Applying result (53) to the latter then yields partial differential equation (48), the direct integration of which readily yields (49). Since $L_c(\rho_c) \triangleq \frac{\rho_c}{O_c(\rho_c)}\frac{\partial O_c(\rho_c)}{\partial \rho_c}$, (49) integrates explicitly to (50). This result also stands for any degenerate state of multiplicity M_j, where for each radioactive width $\boldsymbol{r_j^m}$ we have

$$\frac{r_{j,c}^m(a_c)}{r_{j,c}^m\big(a_c^{(0)}\big)} = \frac{O_c(\rho_c(a_c))}{O_c\big(\rho_c\big(a_c^{(0)}\big)\big)}\sqrt{\frac{a_c^{(0)}}{a_c}}. \tag{57}$$

Finally, the proof of (51) is the element-wise integration of (49) using the Mittag-Leffler pole expansion (7) of $L_c(\rho)$, which we established in Theorem 1 of Ref. [22]—invoking Fubini's theorem to permute sum and integral. In the case of neutral particles, there is a finite number of roots $\{\omega_n\}$ so that the product in Eq. (51) is finite. Note that in the charged-particle case, there is an infinite number (countable) of roots $\{\omega_n\}$, and the Weierstrass factorization theorem would thus usually require (51) to be cast in a Hadamard canonical representation with Weierstrass elementary factors. However, in Eq. (51), the product elements tend toward unity as n goes to infinity $(\frac{k_c a_c - \omega_n}{k_c a_c^{(0)} - \omega_n}) \underset{n\to\infty}{\longrightarrow} 1$, so that the infinite product in Eq. (51) should still converge. ■

Note that for neutral particles (massive or massless) s waves ($\ell = 0$), the outgoing wave function is $O_c(\rho(a_c)) = \mathrm{e}^{\mathrm{i}k_c a_c}$ (cf. Table I of Ref. [22]), so that (50) yields $r_{j,c}(a_c) = r_{j,c}(a_c^{(0)})\sqrt{\frac{a_c^{(0)}}{a_c}}\,e^{ik_c(a_c - a_c^{(0)})}$. Alternatively, directly integrating (49) with the outgoing-wave reduced logarithmic derivative expression $L_c(\rho(a_c)) = ik_c a_c$ yields the same result. Thus, for s-wave neutral channels subject to a change of channel radius, the modulus of the radioactive widths decreases proportionally to the inverse square root of the channel radius a_c, at least for real wave numbers $k_c \in \mathbb{R}$, i.e., real energies above the channel threshold. Since the transition probability rates partial widths can be defined as the square of the modulus of the radioactive width (cf. Eq. (6) in Ref. [57]), this means these transition partial widths decrease inversely to the channel radius: $|\frac{r_{j,c}(a_c)}{r_{j,c}(a_c^{(0)})}|^2 = \frac{a_c^{(0)}}{a_c}$.

A striking property of the R-matrix parametrizations is that they separate the channel contribution to each resonance, meaning that to compute, for instance, the $R_{c,c'}$ element in Eq. (5), one only requires the widths for each level of each

channel, $\gamma_{\lambda,c}$, and not some new parameter for each specific channel pair c, c' combination. In this spirit, we show in Theorem 2 that the Siegert-Humblet radioactive widths $r_{j,c}$ play a similar role in that their transformation under a change of channel radius only depends on that given channel.

Theorem 2 makes explicit the behavior of the radioactive widths $\{r_{j,c}\}$ under a change of channel radius a_c. Strikingly, only the Kapur-Peierls matrix $\boldsymbol{R}_L$ appears in this change of variable. This means that the R-matrix $\boldsymbol{R}$ and the $\boldsymbol{L}^{\boldsymbol{0}}$ matrix function suffice to both compute the Siegert-Humblet parameters $\{\mathcal{E}_j, r_{j,c}\}$ from (11) and to change the radioactive widths $\{r_{j,c}\}$ under a change of channel radius a_c. This result portrays the Siegert-Humblet parameters as allowing a simple energy dependence to the scattering matrix (41)—albeit locally and needing the expansion coefficients (43)—all the while being boundary condition B_c independent and easy to transform under a change of channel radius a_c.

IV. SCATTERING MATRIX CONTINUATION TO COMPLEX ENERGIES

In Sec. 5.2 of Ref. [28], Humblet and Rosenfeld continue the scattering matrix to complex wave numbers $k_c \in \mathbb{C}$ and define corresponding open and closed channels. However, they never point to the conundrum that this entails: In their approach, the scattering matrix seemingly does not annul itself below threshold. This is contrary to the approach taken by Lane and Thomas, where they explicitly annul the elements of the scattering matrix below thresholds, as stated in the paragraph between Eqs. (2.1) and (2.2) of Sec. VII.1, p. 289, in Ref. [2]. Bloch ingeniously circumvents the problem by explicitly stating after Eq. (50) in Ref. [18] that the scattering matrix is a matrix of the open channels only, meaning its dimensions change as more channels open when energy E increases past new thresholds $E > E_{T_c}$. In his approach, subthreshold elements of the scattering matrix need not be annulled; one simply does not consider them.

We dedicate this section to this question of how to extend the scattering matrix to complex wave numbers $k_c \in \mathbb{C}$, while closing the channels below threshold. We argue that analytic continuation of R-matrix operators (Lemma 2 in Sec. III.B of Ref. [22]) is the physically correct way of constructing the scattering matrix for complex wave numbers. To support this, we advance and demonstrate three arguments: Analytic continuation cancels out spurious poles otherwise introduced by the outgoing wave functions O_c (Theorem 3); analytic continuation respects generalized unitarity (Theorem 4); and, for massive particles (not photons), analytic continuation of real wave-number expressions to subthreshold energies naturally sees the transmission matrix evanesce on the physical sheet (Theorem 5), while always closing the channels by annulling the cross section (Theorem 6).

A. Forcing subthreshold elements to zero: The legacy of Lane and Thomas

To close the channels for real energies below threshold, the simplest approach is the one proposed by Lane and Thomas in Ref. [2]. The scattering matrix expressions (2) can be rewritten, for real energies above threshold, according to Sec. VII.1 Eq. (1.6b) in Ref. [2]:

$$\boldsymbol{U} = \boldsymbol{\Omega}(\mathbb{I} + \boldsymbol{w}\boldsymbol{\mathfrak{P}}^{1/2}\boldsymbol{R}_L\boldsymbol{\mathfrak{P}}^{1/2})\boldsymbol{\Omega} \tag{58}$$

with Wronskian $\boldsymbol{w}$ from (3) and the values defined for energies above the thresholds in Sec. III.3.a, p. 271, of Ref. [2]:

$$\begin{aligned} \boldsymbol{\Omega} &\triangleq \boldsymbol{O}^{-1}\boldsymbol{I}, \\ \boldsymbol{\mathfrak{P}} &\triangleq \boldsymbol{\rho}\boldsymbol{O}^{-1}\boldsymbol{I}^{-1}. \end{aligned} \tag{59}$$

Let us note that the Mittag-Leffler expansion (10) of the Kapur-Peierls matrix $\boldsymbol{R}_L$ operator can still be performed.

The Lane and Thomas subthreshold channel force-closure approach exploits the ambiguity in the definition of the shift $\boldsymbol{S}(E)$ and penetration $\boldsymbol{P}(E)$ factors,

$$\boldsymbol{L} = \boldsymbol{S} + i\boldsymbol{P}, \tag{60}$$

for complex energies $E \in \mathbb{C}$, as discussed in Sec. III.B of Ref. [22] (of which we follow the notation). Lane and Thomas choose the branch-point definitions for the shift $\boldsymbol{S}$ and penetration $\boldsymbol{P}$ functions, made explicit in Lemma 1, Sec. III.B, of Ref. [22]. Lane and Thomas do not specify how they would continue the quantities (59) for negative energies, as they state "we need not be concerned with stating similar relations for the negative energy channels" [cf. paragraph after Eq. (4.7c), p. 271], but they do specify that $\boldsymbol{P} = \boldsymbol{0}$ below threshold energies and $\boldsymbol{P} = \boldsymbol{\mathfrak{P}}$ above. This means that plugging in $\boldsymbol{P}$ in place of $\boldsymbol{\mathfrak{P}}$ in Eq. (59) has the convenient property of automatically closing the reaction channels below threshold, since in that case $U_{c,c'} = \Omega_c\Omega_{c'}$, which annuls the off-diagonal terms of the cross section (the reaction channels $c \neq c'$) when plugged into Eq. (1.10) in Ref. [2] VIII.1, p. 291. Note that this approach only annuls the off-diagonal terms of the scattering cross section, leaving nonzero cross sections for the diagonal $\sigma_{cc}(E)$, even below threshold. Indeed, Eq. (4.5a) in Sec. III.4.a, p. 271, of Ref. [2] gives $\Omega_c = e^{i(\omega_c - \phi_c)}$, while the cross section is begotten by the amplitudes of the *transmission matrix* $\boldsymbol{T}(E)$, defined as $T_{cc'} \triangleq \delta_{cc'}\mathrm{e}^{2\mathrm{i}\omega_c} - U_{cc'}$ in (2.3), Sec. VIII.2, p. 292. For subthreshold real energies, the diagonal term of the transmission matrix is thus equal to $T_{cc} = \mathrm{e}^{2\mathrm{i}\omega_c}(1 - \mathrm{e}^{-2\mathrm{i}\phi_c})$. This means that in the Lane and Thomas approach, all channels $c' \neq c$ are force closed to zero below the incoming channel threshold $E < E_{T_c}$, except for the $c \to c$ reaction, which is tactfully overlooked as nonphysical.

Of course, this approach comes at the cost of sacrificing the analytic properties of the scattering matrix $\boldsymbol{U}$: Since $P_c = \mathrm{Im}[L_c]$, the penetration factor is no longer meromorphic and thus neither is $\boldsymbol{U}$. This entails that in decomposition (58) of the scattering matrix, if one "force closes" the channels using the branch-point definition of Lane and Thomas—instead of analytically continuing both $\boldsymbol{\mathfrak{P}}$ and $\boldsymbol{\Omega}$ to complex wave numbers $\boldsymbol{\rho} \in \mathbb{C}$—the scattering matrix $\boldsymbol{U}(E)$ cannot have poles, as there is then no mathematical meaning to such notion. This goes directly against a vast amount of literature on the analytic properties of the scattering matrix [23,24,28–35,37,43,66,67]. This is the approach presently taken by the SAMMY code at Oak Ridge National Laboratory [40] and upon which rest numerous ENDF evaluations [9].

We would like to note that this might not actually have been the approach intended by Lane and Thomas in Ref. [2].

Indeed, Lane and Thomas never specify how to prolong the $\mathfrak{P}$ to subthreshold energies, and in Eq. (58) it is $\mathfrak{P}$ that is present and not $\boldsymbol{P}$. They do, however, note in the paragraph between Eqs. (2.1) and (2.2) of Sec. VII.1, p. 289, that "as there are no physical situations in which the I_c^- occur, the components of the [scattering matrix] are not physically significant and one might as well set them equal to zero as can be seen from (1.6b). This may be accomplished without affecting the [positive energy channels] by setting the negative energy components of the Wronskian matrix to zero; $w_c^- = 0$. (This means that the O_c^- and I_c^- are not linearly independent.)" The choice of wording is here important. Indeed, it says that it is possible to set the Wronskian to zero to close channels below the threshold, though it is not necessary. This is yet another way of closing subthreshold channels that would keep the analytic properties of the scattering matrix, with $\mathfrak{P} \triangleq \boldsymbol{\rho O}^{-1}\boldsymbol{I}^{-1}$ still analytically continued, albeit at the cost of not knowing when in the complex plane the Wronskian w_c should be set to zero—perhaps only on $\mathbb{R}_-$, which would then become a branch line.

We show in Theorem 3 (Sec. IV D) that as long as the Wronskian relation (3) is guaranteed, the poles of the outgoing scattering wave function O_c cancel out of the scattering expressions (2) and (58). The Wronskian condition (3) is conserved when keeping $\mathfrak{P}$ from (59) analytically continued—instead of the definition $P_c \triangleq \mathrm{Im}[L_c]$, which cannot respect the Wronskian relation (3)—so that this approach of setting the Wronskian to zero below threshold while analytically continuing the penetration and shift factors would indeed cancel out the spurious poles of the outgoing wave functions O_c.

B. Analytic continuation of the scattering matrix

In opposition to the Lane and Thomas approach, an entire field of physics and mathematics has studied the analytic continuation of the scattering matrix to complex wave numbers $k_c \in \mathbb{C}$ [23–35].

As we saw, there is no ambiguity as to how to continue the $\boldsymbol{L}(\boldsymbol{\rho})$ matrix function to complex wave numbers (cf. Theorem 1 in Sec. II.B of Ref. [22]), and thus the $\boldsymbol{R}_L$ Kapur-Peierls operator (4). Indeed, the incoming $I_c(\rho_c)$ and outgoing $O_c(\rho_c)$ wave functions can be analytically continued to complex wave numbers $k_c \in \mathbb{C}$ (cf. Theorem 1 in Sec. II.B of Ref. [22]), and through the multisheeted mapping (1) to complex energies $E \in \mathbb{C}$. This naturally yields the meromorphic continuation of the scattering matrix to complex energies (41). Since many evaluations are performed using decomposition (58), in practice performing analytic continuation of R-matrix operators thus means continuing (59) operators $\boldsymbol{\Omega}$ and $\mathfrak{P}$, setting $\mathfrak{P} \triangleq \boldsymbol{P}$, and defining the shift $S_c(\rho_c)$ and penetration $P_c(\rho_c)$ functions as analytically continued complex meromorphic functions (that is definition (44) and Lemma 2 of Ref. [22] as opposed to the Lane and Thomas "force closure" definition (41) and Lemma 1 of Ref. [22]).

The shortcoming of this analytic continuation approach is that it does not evidently annul the channel elements of the scattering matrix for subthreshold energies $E < E_{T_c}$. Indeed, analytic continuation (41) means the scattering matrix $\boldsymbol{U}$ is a meromorphic operator from $\mathbb{C}$ to $\mathbb{C}$ on the multisheeted Riemann surface of mapping (1). Unicity of the analytic continuation then means that if the scattering matrix elements are zero below their threshold, $U_{c,c'}(E) = 0\ ,\ \forall E - E_{T_c} \in \mathbb{R}_-$, then it is identically zero for all energies on that sheet of the manifold: $U_{c,c'}(E) = 0\ ,\ \forall E \in \mathbb{C}$. Thus, the analytic continuation formalism cannot set elements of the scattering matrix to be identically zero below thresholds $\{E_{T_c}\}$.

This apparent inability to close channels below thresholds is the principal reason why the nuclear data community has stuck to the legacy approach of Lane and Thomas (Lemma 1 in Sec. III.B of Ref. [22]), when computing the scattering matrix in Eq. (2). This has been the subject of an ongoing controversy in the field on how to continue the scattering matrix to complex wave numbers.

C. Assuming semisimple poles in *R*-matrix theory

Before advancing our analytic continuation arguments of channel closure (Sec. IV F) and generalized unitarity (Sec. IV E), let us first start with a general note on high-order poles in R-matrix theory (see the consequences for analytic continuation in Sec. IV D). Being a high-order pole, as opposed to a simple pole, can bear various meanings. In our context, the three following definitions are of interest: (a) *Laurent order*, the order of the polar expansion in the Laurent development in the vicinity of a pole; (b) *algebraic multiplicity*, the multiplicity of the root of the resolvant at a pole value; and (c) *geometric multiplicity*, the dimension of the associated null space.

From Eq. (9) and throughout the article, we have treated the case of degenerate states where the geometric multiplicity $M_j > 1$ was higher than one, leading to rank-M_j residues. We have, however, always assumed the Laurent order to be one: In Eq. (9), the residues might be rank M_j, but the Laurent order is still unity (no $\frac{1}{(E-\mathcal{E}_j)^2}$ or higher Laurent orders).

In the general case, the Laurent order is greater than one but it does not equal geometric or algebraic multiplicity. In terms of Jordan normal form, if the Jordan cells had sizes $n_1, ..., n_{m_g}$, then the geometric multiplicity is equal to m_g, the algebraic multiplicity m_a is the sum $m_a = n_1 + \cdots + n_{m_g}$, and the Laurent order is the maximum $\max\{n_1, ..., n_m\}$.

Alternatively, these can be defined as follows: Let $\boldsymbol{M}(z)$ be a complex-symmetric meromorphic matrix operator, with a root at $z = z_0$ (i.e., $\boldsymbol{M}(z_0)$ is noninvertible). The algebraic multiplicity m_a is the first nonzero derivative of the determinant, i.e., the first integer $m_a \in \mathbb{N}$ such that $\frac{d^{m_a}}{dz^{m_a}}\det(\boldsymbol{M}(z))|_{z=z_0} \neq 0$; alternatively, using Cauchy's theorem, the first integer m_a such that $\oint_{\mathcal{C}_{z_0}} \frac{\boldsymbol{M}(z)}{(z-z_0)^{m_a}} dz = \boldsymbol{0}$. The geometric multiplicity m_g is the dimension of the kernel (null space), i.e., $m_g = \dim(\mathrm{Ker}(\boldsymbol{M}(z_0)))$. In general, the algebraic multiplicity is greater than the geometric one: $m_a \geqslant m_g$.

$\boldsymbol{M}(z_0)$ is said to be *semisimple* if its geometric and algebraic multiplicities are equal, i.e., $m_a = m_g$ (cf. Theorem 2, p. 120, in Ref. [68]). Semisimplicity can be established using the following result: $\boldsymbol{M}(z_0)$ is semisimple if and only if for each nonzero $v \in \mathrm{Ker}(\boldsymbol{M}(z_0))$, there exists $w \in \mathrm{Ker}(\boldsymbol{M}(z_0))$ such that

$$v^\mathsf{T}\left(\left.\frac{d\boldsymbol{M}}{dz}\right|_{z=z_0}\right)w \neq 0. \tag{61}$$

If an operator $\boldsymbol{M}(z_0)$ is semisimple at a root z_0, then z_0 is a pole of Laurent order 1 for the inverse operator $\boldsymbol{M}^{-1}(z) \underset{\mathcal{W}(z_0)}{\sim} \frac{\widetilde{\boldsymbol{M}}}{z-z_0}$. For Hermitian operators, the semisimplicity property is guaranteed. However, resonances seldom correspond to Hermitian operators. In our case, the resonances correspond to the poles of the scattering matrix $\boldsymbol{U}(E)$, which is not self-adjoint but complex symmetric $\boldsymbol{U}^{\mathsf{T}} = \boldsymbol{U}$ (cf. Eq. (2.15), Sec. VI.2.c, p. 287, in Ref. [2]). For complex-symmetric operators, semisimplicity is not guaranteed in general, even when discarding the complex case of quasinull vectors.

In the case of R-matrix theory, we were able to find cases where the geometric multiplicity of the scattering matrix does not match the algebraic one, thus R-matrix theory does not always yield semisimple scattering matrices, and the Laurent development orders of the resonance poles can be higher. For instance, we can devise examples of nonsemisimple inverse level matrices from definition (8) by choosing resonance parameters such that the algebraic multiplicity is strictly greater than the geometric one.

However, one can also observe in these simple cases that the space of parameters for which semisimplicity is broken is a hyperplane of the space of R-matrix parameters. This gives credit to the traditional physics arguments that the probability of this occurring is quasinull: R-matrix theory can yield scattering matrices with Laurent orders higher than one, but this is extremely unlikely; a mathematical approach of generic simplicity of resonances can be found in Chap. 4 of Ref. [23], in particular, Theorems 4.4, 4.5, 4.7, and 4.39. In other terms, we assume semisimplicity is almost always guaranteed through R-matrix parametrizations.

Henceforth, we use this argument to continue assuming the Kapur-Peierls matrix $\boldsymbol{R}_L$ is usually semisimple, and thus the Laurent order of the radioactive poles $\{\mathcal{E}_j\}$ in Eq. (9) is, in practice, one.

Let us be aware that in general scattering theory, the scattering operator may exhibit high-order poles [23,24,69], and efforts are being made to have these "exceptional points" of second order arise in the specific case of nuclear interactions [70,71]. The traditional R-matrix assumption where the poles of the scattering matrix are almost always of Laurent order 1 is unable to describe these physical phenomena.

D. Scattering matrix poles are the Siegert-Humblet radioactive poles

This section is dedicated to a remarkable property of the Siegert-Humblet radioactive poles $\{\mathcal{E}_j\}$: In R-matrix theory, these are exactly the poles of the scattering matrix (Theorem 3).

Theorem 3. SCATTERING MATRIX POLES ARE THE SIEGERT-HUMBLET RADIOACTIVE POLES.

In R-matrix theory, when the R-matrix operators (Kapur-Peierls $\boldsymbol{R}_L$ and incoming and outgoing wave functions $\boldsymbol{I}$ and $\boldsymbol{O}$) are analytically continued to complex energies $E \in \mathbb{C}$ such as with respect to the Wronskian condition (3), then the poles of the scattering matrix $\boldsymbol{U}$ are exactly the poles of the Kapur-Peierls operator $\boldsymbol{R}_L$, i.e., the Siegert-Humblet radioactive poles $\{\mathcal{E}_j\}$ from (11) and (12). These poles are almost always of Laurent order 1.

Section IV C gives the reasons to assume that the poles of the Kapur-Peierls matrix $\boldsymbol{R}_L$ are simple (i.e., Laurent order 1). For the rest of this theorem, we here give two proofs: a first proof by *reductio ad absurdum* and a second constructive proof.

Proof. Reductio ad absurdum. Since the radioactive poles $\mathcal{E}_j$ are not poles of the outgoing wave function, i.e., $\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}(\mathcal{E}_j) \neq \boldsymbol{0}$, expression (2) implies that all the poles $\mathcal{E}_j$ of the Kapur-Peierls $\boldsymbol{R}_L(E)$ operator are poles of the scattering matrix $\boldsymbol{U}(E)$. As first sight, expression (2) would suggest the roots $\{\omega_n\}$ of the outgoing wave functions (i.e., all such that there exists a channel c for which $O_c(\omega_n) = 0$) are also poles of the scattering matrix. However, when performing analytic continuation of R-matrix operators while conserving the Wronskian condition (3), expression (2) is equivalent to Eq. (1.5) of Sec. VII.1 of Ref. [2], for which it is evident that the roots $\{\omega_n\}$ of the outgoing wave function $O_c(\rho_c)$ are not poles of the scattering matrix $\boldsymbol{U}$ [that is because in both the Coulomb and the neutral-particle case the outgoing wave functions $O_c(\rho_c)$ are confluent hypergeometric functions with simple roots $\{\omega_n\}$ entailing that $O_c^{(1)}(\omega_n) \neq 0$]. Hence, the poles of the scattering matrix $\boldsymbol{U}(E)$ must be exactly all the radioactive poles $\mathcal{E}_j$. ■

Though this latter proof is correct, it does not explain how the roots $\{\omega_n\}$ of the outgoing wave function $O_c(\rho_c)$ cancel out of the scattering matrix in expression (2). It is important to understand this because expression (2) defines the potential cross section in standard nuclear data libraries, which taken as is should thus count the $\{\omega_n\}$ as poles. We use this explicit cancellation of these spurious poles at the residue level to establish the windowed multipole representation in our followup article [36]. Moreover, if one uses the Lane and Thomas "force closure" definitions, then expression (2) and Eq. (1.5) of Sec. VII.1 of Ref. [2] are no longer equivalent in the complex plane. In this case, not only is the scattering matrix $\boldsymbol{U}(E)$ no longer meromorphic, but it also diverges at the $\{\omega_n\}$ outgoing wave-function roots. Also, a constructive proof requires a closer look at the behavior of specific poles and residues and gives us an opportunity to explain in detail different nontrivial assumptions usually made in nuclear physics about radioactive states and other states' degeneracy. For all these reasons, we believe it of interest to here provide a second, constructive proof of Theorem 3. It rests on the following Lemma 1.

Lemma 1. DIAGONAL SEMISIMPLICITY. If a diagonal matrix $\boldsymbol{D}^{-1}(z)$ is composed of elements with simple roots $\{\omega_n\}$, then its inverse is semisimple, i.e., when a pole ω_n of a diagonal matrix $\boldsymbol{D}(z)$ has an algebraic multiplicity $M_n > 1$ the Laurent development order of the pole remains 1 while the associated residue matrix is of rank M_n and can be expressed as

$$\boldsymbol{D}(z) \underset{\mathcal{W}(z=\omega_n)}{=} \boldsymbol{D}_0 + \frac{\boldsymbol{D}_n}{z-\omega_n},$$
$$\boldsymbol{D}_n \triangleq \sum_{m=1}^{M_n} \frac{\boldsymbol{v_n}\boldsymbol{v_n}^{\mathsf{T}}}{\boldsymbol{v_n}^{\mathsf{T}}\boldsymbol{D_0^{-1}}^{(1)}\boldsymbol{v_n}}. \tag{62}$$

Proof. Without loss of generality, a change of variables can be performed so as to set $\omega_n = 0$. Let $\boldsymbol{D}(z) = \mathbf{diag}(d_1(z), d_2(z), \ldots, d_1(z), d_j(z), d_n(z))$ be a diagonal meromorphic complex-valued operator, which admits a pole at $z = 0$. $\boldsymbol{D^{-1}}(z) = \mathbf{diag}(d_1^{-1}(z), d_2^{-1}(z), \ldots, d_1^{-1}(z), d_j^{-1}(z), d_n^{-1}(z))$ is well known, and $\det(\boldsymbol{D^{-1}})(z=0) = d_1^{-1}(z)^2 \prod_{j\neq 1} d_j^{-1}(z)$. Let us assume only $d_1^{-1}(z=0) = 0$, with a simple root, so that $d_1(z) \underset{\mathcal{W}(z=0)}{=} d0_1 + \frac{R_1}{z}$. Then $\det(\boldsymbol{D^{-1}}(z))(z=0) = d_1^{-1}(z)^2 \prod_{j\neq 1} d_j^{-1}(z)$ has a double root: The algebraic multiplicity is thus 2. However, it is immediate to notice that

$$\begin{aligned}\boldsymbol{D}(z) &= \mathbf{diag}(d_1(z), d_2(z), \ldots, d_1(z), d_j(z), d_n(z)) \\ &\underset{\mathcal{W}(z=0)}{=} \mathbf{diag}(d0_1, d_2(z), \ldots, d0_1(z), d_j(z), d_n(z)) \\ &\quad + \frac{1}{z}\mathbf{diag}(R_1, 0, \ldots, R_1, 0, 0).\end{aligned}$$

This means the Laurent development order remains 1, albeit the algebraic multiplicity of the pole is 2 (or higher M_n). It can thus be written that $\boldsymbol{D}(z) \underset{\mathcal{W}(z=0)}{=} \boldsymbol{D_0} + \frac{\boldsymbol{D_1}}{z}$. When solving for the nonlinear eigenproblem $\boldsymbol{D^{-1}}(z)\boldsymbol{v} = \boldsymbol{0}$, the kernel is no longer an eigenline, but instead spans $(\boldsymbol{v_1}, \boldsymbol{v_2})$, i.e., $\mathrm{Ker}(\boldsymbol{D^{-1}}_0) = \mathrm{Span}(\boldsymbol{v_1}, \boldsymbol{v_2})$, with $\boldsymbol{v_1} = a_1[1, 0, \ldots, 0, 0, 0]^\mathsf{T}$ and $\boldsymbol{v_2} = a_2[0, 0, \ldots, 1, 0, 0]^\mathsf{T}$. Then, following Gohberg-Sigal's theory [49], the fundamental property

$$\boldsymbol{D^{-1}D} = \mathbb{I}$$

and the Laurent development around the pole

$$\boldsymbol{D^{-1}}(z) \underset{\mathcal{W}(z=0)}{=} \boldsymbol{D_0^{-1}} + z\boldsymbol{D_0^{-1}}^{(1)} + \mathcal{O}(z^2)$$

yield the relations

$$\begin{aligned}\boldsymbol{D_0^{-1}D_0} + \boldsymbol{D_0^{-1}}^{(1)}\boldsymbol{D_1} &= \mathbb{I}, \\ \boldsymbol{D_0^{-1}D_1} &= \boldsymbol{0}.\end{aligned}$$

Constructing $\boldsymbol{D_1}$ to satisfy the latter then entails

$$\boldsymbol{D_1} = \frac{\boldsymbol{v_1 v_1^\mathsf{T}}}{\boldsymbol{v_1^\mathsf{T} D_0^{-1}}^{(1)}\boldsymbol{v_1}} + \frac{\boldsymbol{v_2 v_2^\mathsf{T}}}{\boldsymbol{v_2^\mathsf{T} D_0^{-1}}^{(1)}\boldsymbol{v_2}},$$

where the transpose is used because the matrix is complex symmetric. This reasoning immediately generalizes to expression (62). ■

Let $\{\omega_n\}$ be all the roots of the outgoing wave functions (i.e., the poles of inverse outgoing wave $\boldsymbol{O^{-1}}$), which we can find by solving the nonlinear eigenvalue problem:

$$\boldsymbol{O}(\omega_n)\boldsymbol{w_{nm}} = \boldsymbol{0}. \tag{63}$$

Looking at (2) shows that the roots of the outgoing wave functions $\boldsymbol{O}$ could endow the scattering matrix with additional poles, through $\boldsymbol{O^{-1}}$, and that these poles could potentially have higher Laurent orders, since $\boldsymbol{O^{-1}}$ appears twice in expression (2). Yet, because $\boldsymbol{O}$ is diagonal with simple roots, lemma 1 entails $\boldsymbol{O^{-1}}$ is semisimple: The algebraic multiplicities are equal to the geometric multiplicities, and thus the poles $\{\omega_n\}$ all have Laurent order 1. Situations can arise where same-charge channels within the same total angular momentum J^π will carry same angular momenta $\ell_c = \ell_{c'}$ and equal channel radii $a_c = a_{c'}$. In that case, the geometric multiplicity M_n of pole ω_n will be equal to the number of channels sharing the same functional outgoing waves $O_c = O_{c'}$. Diagonal semisimplicity lemma 1 then establishes that the residue of $\boldsymbol{O^{-1}}$ associated to pole ω_n is now a diagonal rank-M_n matrix, $\boldsymbol{D_n}$, expressed as

$$\boldsymbol{D_n} = \sum_{m=1}^{M_n} \frac{\boldsymbol{w_{nm} w_{nm}^\mathsf{T}}}{\boldsymbol{w_{nm}^\mathsf{T} O}^{(1)}(\omega_n)\boldsymbol{w_{nm}}}, \tag{64}$$

where $\boldsymbol{O}^{(1)}(\omega_n)$ designates the first derivative of $\boldsymbol{O}$, evaluated at the pole value ω_n. This establishes the existence of higher rank residues associated to the inverse outgoing wave function $\boldsymbol{O^{-1}}$. Notice that if the channel radii $\{a_c\}$ were chosen at random, these high-rank residues would almost never emerge (null probability). However, since a_c is chosen arbitrarily in the context of R-matrix theory, it is often the case that evaluators set a_c to a fixed value for multiple different channels and even across isotopes. This is because the scattering radius is determined early on by the evaluator (and not varied afterward) based on the amount of potential scattering observed in the experimental data, which is very similar for isotopes of the same element. Therefore, in practice these high-rank residues are not uncommon. Our constructive proof now establishes how analytic continuation annuls these high-rank residues.

Proof. Constructive. Consider the scattering matrix expression $\boldsymbol{U} = \boldsymbol{O^{-1}}[\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{R_L O^{-1}}\boldsymbol{\rho}^{1/2}]$ from (2). Result (64) entails that, in the vicinity of ω_n (root of the outgoing wave function $\boldsymbol{O}$) the residue is locally given by

$$\boldsymbol{U}(z) \underset{\mathcal{W}(E=\omega_n)}{=} \boldsymbol{U}_0(\omega_n) + \frac{\boldsymbol{D_n}[\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{R_L O^{-1}}\boldsymbol{\rho}^{1/2}]_{E=\omega_n}}{E - \omega_n}. \tag{65}$$

We now notice that evaluating the Kapur-Peierls $\boldsymbol{R_L}$ operator (4) at the pole value ω_n yields the following equality:

$$\boldsymbol{R_L O^{-1}}(\omega_n)\boldsymbol{w_{nm}} = -[\boldsymbol{\rho O}^{(1)}]^{-1}(\omega_n)\boldsymbol{w_{nm}}. \tag{66}$$

Plugging (66) into the residue of (65), and using the fact that (64) guarantees $\boldsymbol{D_n}$ is a linear combination of $\boldsymbol{w_{nm} w_{nm}^\mathsf{T}}$, we then have the following equality on the residues at poles ω_n:

$$\boldsymbol{D_n}[\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{R_L O^{-1}}\boldsymbol{\rho}^{1/2}]_{E=\omega_n} = \boldsymbol{D_n}[\boldsymbol{I} - 2i\boldsymbol{O}^{(1)^{-1}}]_{E=\omega_n}. \tag{67}$$

The right-most term is diagonal and independent from the resonance parameters. Since the Wronskian matrix $\boldsymbol{w}$ of the external region interaction (for Coulomb or free particles) is constant (3), $\boldsymbol{w} = \boldsymbol{O}^{(1)}\boldsymbol{I} - \boldsymbol{I}^{(1)}\boldsymbol{O} = 2i\mathbb{I}$, evaluating at outgoing wave-function root ω_n, one finds $2i\mathbb{I} = \boldsymbol{O}^{(1)}\boldsymbol{I}(\omega_n)$. Plugging this result into (67) annuls the corresponding residue from the scattering matrix, i.e.,

$$\boldsymbol{D_n}[\boldsymbol{I} + 2i\boldsymbol{\rho}^{1/2}\boldsymbol{R_L O^{-1}}\boldsymbol{\rho}^{1/2}]_{E=\omega_n} = \boldsymbol{0}. \tag{68}$$

Thus, if the Wronskian condition (3) is respected, the $\{\omega_n\}$ poles cancel out of the scattering matrix $\boldsymbol{U}$. ■

Importantly, both the Lane and Thomas force closing of subthreshold channels IV A or the analytic continuation IV B will yield the same cross-section values for real energies

above thresholds. However, Theorem 3 demonstrates that the choice of analytic continuation in Eq. (2), respecting the Wronskian condition (3), leads to the cancellation from the scattering matrix $\boldsymbol{U}$ of the $\{\omega_n\}$ spurious poles, which have nothing to do with the resonant states of the scattering system. This cancellation is thus physically accurate and would not take place had the choice of $\mathfrak{P} = \boldsymbol{P}$ been made in Eq. (58) with the Lane and Thomas "force closure" definition $\boldsymbol{P} = \mathrm{Im}[\boldsymbol{L}(z)] \in \mathbb{R}$ (cf. Lemma 1 in Sec. III.B of Ref. [22]), under which the scattering matrix diverges at $\{\omega_n\}$. Conversely, analytically continuing the penetration function as $\boldsymbol{P}(z) \triangleq \frac{1}{2\mathrm{i}}(\boldsymbol{L}(z) - [\boldsymbol{L}(z^*)]^*) \in \mathbb{C}$ (cf. Lemma 2 in Sec. III.B of Ref. [22]) will guarantee the cancellation of the $\{\omega_n\}$ poles from the scattering matrix $\boldsymbol{U}$ when using (58). Notice this is almost the definition (74) of $\boldsymbol{\Delta L}(\rho)$ we hereafter use in the proof of the generalized unitarity. Then, to force close subthreshold channels, one could set the Wronskian to zero, as proposed by Lane and Thomas in the paragraph between Eqs. (2.1) and (2.2) of Sec. VII.1, p. 289. This shifts the problem to how to maintain the Wronskian condition (3) while setting the Wronskian to zero below thresholds. Alternatively, we here argue in Sec. IV F that this might not be necessary, as analytic continuation can naturally close subthreshold channels.

E. Generalized unitarity for analytically continued scattering matrix

Hale proved a more esoteric argument in favor of analytic continuation of the scattering matrix, showing it satisfies generalized unitarity.

Eden and Taylor established a generalized unitarity condition, Eq. (2.16) in Ref. [37], which extents the one described by Lane and Thomas, Eq. (2.13), Sec. VI.2.c, p. 287, in that the subset of open channels is unitary (thus conserving probability), but the scattering matrix can still be continued to subthreshold channels and be nonzero; that is, the full scattering matrix of open and closed channels is not unitary but satisfies the generalized unitarity condition. This is also consistent with approaches other than R matrix to modeling nuclear interactions (cf. commentary above Eq. (3), p. 4 in Ref. [71], and Refs. [25,27]).

The premises of the problem lies again in the multisheeted Riemann surface spawning from mapping (1): When considering the scattering matrix $\boldsymbol{U}(E)$ at a given energy E, there are multiple possibilities for the choice of wave number k_c at each channel. Following Eden and Taylor's Eqs. (2.14a) and (2.14b) [37], we consider the case of momenta being continued along the following paths in the multisheeted Riemann surface: One subset of channels c, denoted by $\widehat{\mathfrak{C}}$, is continued as $k_{c\in\widehat{\mathfrak{C}}} \to k^*_{c\in\widehat{\mathfrak{C}}}$, while all the others are continued as $k_{c\notin\widehat{\mathfrak{C}}} \to -k^*_{c\notin\widehat{\mathfrak{C}}}$, and we collectively denote this continuation $\boldsymbol{k} \to \widetilde{\boldsymbol{k}}$:

$$\boldsymbol{k} \to \widetilde{\boldsymbol{k}} : \begin{cases} \forall c \in \widehat{\mathfrak{C}}\,, & k_c \to k_c^* \\ \forall c \notin \widehat{\mathfrak{C}}\,, & k_c \to -k_c^*. \end{cases} \tag{69}$$

We then seek to reproduce the generalized unitarity property, Eq. (2.16) of Ref. [37], which states that the submatrix $\widehat{\boldsymbol{U}}$ composed of the channels $c \in \widehat{\mathfrak{C}}$ verifies the generalized unitarity condition:

$$\widehat{\boldsymbol{U}}(\boldsymbol{k})[\widehat{\boldsymbol{U}}(\widetilde{\boldsymbol{k}})]^\dagger = \mathbb{I}. \tag{70}$$

We now show that analytically continuing the R-matrix expression (2) ensures the scattering matrix and respects Eden and Taylor generalized unitarity condition.

Theorem 4. ANALYTIC CONTINUATION OF THE R-MATRIX EXPRESSION FOR THE SCATTERING MATRIX ENSURES GENERALIZED UNITARITY.

By performing the analytic continuation of the R-matrix expression (2), the scattering matrix $\boldsymbol{U}$ satisfies Eden and Taylor's generalized unitarity condition (70).

Proof. The proof is based on the conjugacy relations of the outgoing and incoming wave functions, Eq. (2.12), Sec. VI.2.c, in Ref. [2], whereby for any channel c

$$\begin{aligned} [O_c(k_c^*)]^* &= I_c(k_c), \quad [I_c(k_c^*)]^* = O_c(k_c), \\ O_c(-k_c) &= I_c(k_c), \quad I_c(-k_c) = O_c(k_c), \\ -O_c^{(1)}(-k_c) &= I_c^{(1)}(k_c), \quad -I_c^{(1)}(-k_c) = O_c^{(1)}(k_c), \end{aligned} \tag{71}$$

where the third line was obtained by taking the derivative of the second. Conjugacy relations (71) entail the following relations on the outgoing-wave reduced logarithmic derivative $\boldsymbol{L}$:

$$[L_c(k_c^*)]^* = L_c(-k_c), \quad [L_c(-k_c^*)]^* = L_c(k_c). \tag{72}$$

We also notice that the Wronskian condition (3) is equivalent to

$$\frac{2i\rho_c}{O_c I_c} = \rho_c\left[\frac{O_c^{(1)}}{O_c} - \frac{I_c^{(1)}}{I_c}\right]. \tag{73}$$

Recognizing the definition (6) of $\boldsymbol{L}$ and using conjugacy relations (72), this Wronskian condition (73) can be expressed as a difference of the reduced logarithmic L_c derivatives:

$$\Delta L_c(k_c) \triangleq L_c(k_c) - L_c(-k_c) = \frac{2\mathrm{i}\rho_c}{O_c I_c}(k_c). \tag{74}$$

Defining the diagonal matrix $\boldsymbol{\Delta L} \triangleq \mathbf{diag}(\Delta L_c(k_c))$, we can then rewrite, similarly to (58), the R-matrix expression (2) of the scattering matrix $\boldsymbol{U}$ as a function of $\Delta L_c(k_c)$, so that

$$\begin{aligned} \boldsymbol{U} &= \boldsymbol{O}^{-1}[\mathbb{I} + [\boldsymbol{\rho}^{1/2}\boldsymbol{R}_L\boldsymbol{\rho}^{-1/2}]\boldsymbol{\Delta L}]\boldsymbol{I} \\ &= \boldsymbol{I}[\mathbb{I} + \boldsymbol{\Delta L}[\boldsymbol{\rho}^{-1/2}\boldsymbol{R}_L\boldsymbol{\rho}^{1/2}]]\boldsymbol{O}^{-1}. \end{aligned} \tag{75}$$

Notice again how this expression is closely related to the analytic continuation of expression (58).

Coming back to the Eden and Taylor continuation (69), let us now establish a relation between the Kapur-Peierls operator $\boldsymbol{R}_L$ and $\boldsymbol{\Delta L}$. From the definition (4) of the Kapur-Peierls operator $\boldsymbol{R}_L$, recalling that under Eden and Taylor continuations (69) the energy E from mapping (1) remains unaltered, and given that the boundary condition B_c in the $\boldsymbol{L}^{\boldsymbol{0}}$ matrix function is real and thus the R-matrix parameters (5) are too, it follows that

$$\left[\boldsymbol{R}_L^{-1}(\widetilde{\boldsymbol{k}})\right]^* - \boldsymbol{R}_L^{-1}(\boldsymbol{k}) = \begin{pmatrix} \widehat{\boldsymbol{\Delta L}}(\boldsymbol{k}) & 0 \\ 0 & 0 \end{pmatrix}, \tag{76}$$

where we have used the $\boldsymbol{L}$ conjugacy relations (72) to establish that all channels $c \notin \widehat{\mathfrak{C}}$ cancel out, and the rest yield $\Delta L_{c\in\widehat{\mathfrak{C}}}(k_c)$. The $\widehat{\boldsymbol{\Delta L}}$ thus designates the submatrix composed of all the channels $c \in \widehat{\mathfrak{C}}$. Multiplying both left and right and considering the submatrices on the channels $c \in \widehat{\mathfrak{C}}$ thus yield

$$\widehat{\boldsymbol{R}}_L(k) - [\widehat{\boldsymbol{R}}_L(\widetilde{k})]^* = \widehat{\boldsymbol{R}}_L(k)\widehat{\boldsymbol{\Delta L}}(k)[\widehat{\boldsymbol{R}}_L(\widetilde{k})]^*. \tag{77}$$

This relation is what guarantees that the scattering matrix $\boldsymbol{U}$ satisfies generalized unitarity condition (70). Indeed, let us develop the left-hand side of (70), using expressions (75) on the submatrices of the channels $c \in \widehat{\mathfrak{C}}$:

$$\begin{aligned}\widehat{\boldsymbol{U}}(k)\big[\widehat{\boldsymbol{U}}(\widetilde{k})\big]^\dagger &= \widehat{\boldsymbol{O}}^{-1}(k)\big[\mathbb{I} + \big[\widehat{\boldsymbol{\rho}^{\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{-\frac12}}\big](k)\widehat{\boldsymbol{\Delta L}}(k)\big]\widehat{\boldsymbol{I}}(k)\\ &\quad\times\big[\widehat{\boldsymbol{I}}(\widetilde{k})\big[\mathbb{I} + \widehat{\boldsymbol{\Delta L}}(\widetilde{k})\big[\widehat{\boldsymbol{\rho}^{-\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{\frac12}}\big](\widetilde{k})\big]\widehat{\boldsymbol{O}}^{-1}(\widetilde{k})\big]^\dagger\\ &= \widehat{\boldsymbol{O}}^{-1}(k)\big[\mathbb{I} + \big[\widehat{\boldsymbol{\rho}^{\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{-\frac12}}\big](k)\widehat{\boldsymbol{\Delta L}}(k)\big]\widehat{\boldsymbol{I}}(k)\\ &\quad\times[\widehat{\boldsymbol{O}}^{-1}(\widehat{k^*})]^*\big[\mathbb{I}+\big[\widehat{\boldsymbol{\rho}^{-\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{\frac12}}\big](\widehat{k^*})\\ &\quad\times[\widehat{\boldsymbol{\Delta L}}(\widehat{k^*})]^*\big][\widehat{\boldsymbol{I}}(\widehat{k^*})]^*.\end{aligned} \tag{78}$$

Noticing that conjugacy relation (72) entail the following $\boldsymbol{\Delta L}$ symmetry from definition (74), $[\widehat{\boldsymbol{\Delta L}}(\widehat{k^*})]^* = -\widehat{\boldsymbol{\Delta L}}(k)$, and making use of the conjugacy relations for the wave functions (71), we can further simplify (78) to

$$\begin{aligned}\widehat{\boldsymbol{U}}(k)[\widehat{\boldsymbol{U}}(\widetilde{k})]^\dagger &= \mathbb{I} \;+\; \widehat{\boldsymbol{O}}^{-1}(k)\big[\widehat{\boldsymbol{\rho}^{\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{-\frac12}}\big](k)\\ &\quad\times\Big\{\Big[\Big[\widehat{\boldsymbol{\rho}^{\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{-\frac12}}\Big]^{-1}(k^*)\Big]^\dagger\\ &\quad-\Big[\widehat{\boldsymbol{\rho}^{\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{-\frac12}}\Big]^{-1}(k) - \widehat{\boldsymbol{\Delta L}}(k)\Big\}\\ &\quad\times\big[\big[\widehat{\boldsymbol{\rho}^{-\frac12}\boldsymbol{R}_L\boldsymbol{\rho}^{\frac12}}\big](\widehat{k^*})\big]^\dagger\widehat{\boldsymbol{\Delta L}}(k)\widehat{\boldsymbol{O}}(k).\end{aligned} \tag{79}$$

In the middle, we recognize property (76), where the $\boldsymbol{\rho}^{\pm1/2}$ cancel out by commuting with the diagonal matrix. Property (76) thus annuls all nonidentity terms, leaving Eden and Taylor's generalized unitarity condition (70) satisfied. ■

Let us also note that the proof required real boundary conditions $B_c \in \mathbb{R}$. Thus, in R-matrix parametrization (2), real boundary conditions $B_c \in \mathbb{R}$ are necessary for the scattering matrix $\boldsymbol{U}$ to be unitarity (and by extension generalized unitary).

Theorem 4 has a strong argument in favor of performing analytic continuation of the R-matrix operators as the physically correct way of prolonging the scattering matrix to complex wave numbers $k_c \in \mathbb{C}$.

F. Closure of subthreshold cross sections through analytic continuation

We finish this article with the key question of how to close subthreshold channels. Analytically continuing the scattering matrix below thresholds entails it cannot be identically zero there, since this would entail it is the null function on the entire sheet of the manifold (unicity of analytic continuation). However, we here show that for massive particles subject to $\rho(E)$ mappings (2) or (4), Sec. II.A of Ref. [22], adequate definitions and careful consideration will both make the transmission matrix evanescent subthreshold (in a classical case of quantum tunneling) and annul the subthreshold cross section—the physically measurable quantity.

The equations linking the scattering matrix $\boldsymbol{U}$ to the cross section—Eqs. (1.9), (1.10), and (2.4) in Sec. VIII.1. of Ref. [2], pp. 291–293—were only derived for real positive wave numbers. Yet, when performing analytic continuation of them to subthreshold energies, the quantum tunneling effect will naturally make the transmission matrix infinitesimal on the physical sheet of mapping (1). Indeed, the *transmission matrix*, $\boldsymbol{T}$, is defined in Ref. [2] after Eq. (2.3), Sec. VIII.2, p. 292, as

$$T_{cc'} \triangleq \delta_{cc'}\mathrm{e}^{2\mathrm{i}\omega_c} - U_{cc'}, \tag{80}$$

where ω_c is defined by Lane and Thomas in Eq. (2.13c), Sec. III.2.b, p. 269, and used in Eq. (4.5a), Sec. III.4.a, p. 271, in Ref. [2], and is the difference $\omega_c = \sigma_{\ell_c}(\eta_c) - \sigma_0(\eta_c)$, where the *Coulomb phase shift*, $\sigma_{\ell_c}(\eta_c)$ is defined by Thompson in Eq. (33.2.10) of Ref. [72]. Defining the diagonal matrix $\boldsymbol{\omega} \triangleq \mathbf{diag}(\omega_c)$ and using the R-matrix expression (2) for the scattering matrix, the Lane and Thomas transmission matrix (80) can be expressed with R-matrix parameters as

$$\boldsymbol{T}_{\mathrm{L\&T}} \triangleq -2\mathrm{i}\boldsymbol{O}^{-1}\left[\underbrace{\left(\frac{\boldsymbol{I}-\boldsymbol{O}\mathrm{e}^{2\mathrm{i}\boldsymbol{\omega}}}{2\mathrm{i}}\right)}_{\boldsymbol{\Theta}} + \boldsymbol{\rho}^{1/2}\boldsymbol{R}_L\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}\right]. \tag{81}$$

The angle-integrated partial cross sections $\sigma_{cc'}(E)$ can then be expressed as Eq. (3.2d), Sec. VIII.3, p. 293, of Ref. [2]:

$$\sigma_{cc'}(E) = \pi g_{J_c^\pi}\left|\frac{T^{cc'}_{\mathrm{L\&T}}(E)}{k_c(E)}\right|^2, \tag{82}$$

where $g_{J_c^\pi} \triangleq \frac{2J+1}{(2I_1+1)(2I_2+1)}$ is the *spin statistical factor* defined in Eq. (3.2c), Sec. VIII.3, p. 293. Plugging in the transmission matrix R-matrix parametrization (81) into cross-section expression (82) then yields [2]

$$\sigma_{cc'} = 4\pi g_{J_c^\pi}\left|\frac{1}{O_c k_c}\right|^2 |\boldsymbol{\Theta} + \boldsymbol{\rho}^{1/2}\boldsymbol{R}_L\boldsymbol{O}^{-1}\boldsymbol{\rho}^{1/2}|^2_{cc'}. \tag{83}$$

An alternative, more numerically stable, way of computing the cross section is used at Los Alamos National Laboratory, where Hale introduced the following rotated transmission matrix, defined as

$$\boldsymbol{T}_{\mathrm{H}} \triangleq -\frac{\mathbf{e}^{-i\boldsymbol{\omega}}\boldsymbol{T}_{\mathrm{L\&T}}\mathbf{e}^{-i\boldsymbol{\omega}}}{2i} \tag{84}$$

and whose R-matrix parametrization is thus

$$\boldsymbol{T}_{\mathrm{H}} = \boldsymbol{H}_+^{-1}\left[\boldsymbol{\rho}^{1/2}\boldsymbol{R}_L\boldsymbol{\rho}^{1/2}\boldsymbol{H}_+^{-1} - \underbrace{\left(\frac{\boldsymbol{H}_+ - \boldsymbol{H}_-}{2i}\right)}_{\boldsymbol{F}}\right], \tag{85}$$

where $\boldsymbol{H}_\pm$ are defined as in Eqs. (2.13a) and (2.13b), Sec. III.2.b, p. 269, of Ref. [2]:

$$\begin{aligned}H_{+c} &= O_c e^{i\omega_c} = G_c + iF_c,\\ H_{-c} &= I_c e^{-i\omega_c} = G_c - iF_c,\end{aligned} \tag{86}$$

and for which we refer to Eq. (33.2.11) in Ref. [72] and Chapter 14 of Ref. [73]. The partial cross section is then directly related to the $\boldsymbol{T}_{\mathrm{H}}$ rotated transmission matrix (84) as

$$\sigma_{cc'}(E) = 4\pi g_{J_c^\pi} \left| \frac{T_H^{cc'}(E)}{k_c(E)} \right|^2. \tag{87}$$

Theorem 5. EVANESCENCE OF SUBTHRESHOLD TRANSMISSION MATRIX.

For massive particles, analytic continuation of R-matrix parametrization (2) makes the subthreshold transmission matrix $\boldsymbol{T}$, defined as (81), evanescent on the physical sheets of wave-number-energy $\rho(E)$ mappings (2) or (4), Sec. II.A of Eq. [22]. In turn, this quantum tunneling entails the partial cross sections $\sigma_{cc'}(E)$ become infinitesimal below threshold.

Proof. The proof is based on noticing that both transmission matrix expressions (81) and (84) entail their modulus square is proportional to

$$|\boldsymbol{T}_{cc'}|^2(E) \propto \left| \frac{1}{H_+(E)} \right|^2. \tag{88}$$

This is because $\boldsymbol{R}_L \boldsymbol{O}^{-1} = [\boldsymbol{O}[\boldsymbol{R}^{-1} - \boldsymbol{B}] - \boldsymbol{\rho}\boldsymbol{O}^{(1)}]^{-1}$, which does not diverge below threshold. Asymptotic expressions for the behavior of $H_+(\rho)$ then yield, for small ρ values,

$$H_+(\rho) \underset{\rho\to 0}{\sim} \frac{\rho^{-\ell}}{(2\ell+1)C_\ell(\eta)} - iC_\ell(\eta)\rho^{\ell+1} \tag{89}$$

and asymptotic large-ρ behavior

$$H_+(\rho) \underset{\rho\to\infty}{\sim} e^{i(\rho - \eta\ln(2\rho) - \frac{1}{2}\ell\pi + \sigma_\ell(\eta))}. \tag{90}$$

Above the threshold, $\rho \in \mathbb{R}$ is real and thus Eq. (90) shows how $|H_+(\rho)| \underset{\rho\to\infty}{\longrightarrow} 1$. In other terms, the $|H_+(\rho)|$ term cancels out of the cross-section expressions (83) and (87) for open channels above threshold.

Yet, in both wave-number energy $\rho(E)$ mappings (2) or (4) in Sec. II.A of Ref. [22], the subthreshold dimensionless wave number is purely imaginary: $\rho \in \mathrm{i}\mathbb{R}$. Since asymptotic form (90) is dominated in modulus by $|H_+(\rho)| \underset{\rho\to\infty}{\sim} |e^{i\rho}|$. Depending on which sheet ρ is continued subthreshold, we can have $\rho = \pm ix$, with $x \in \mathbb{R}$. Thus, on the nonphysical sheet $\{E, \ldots, -_c, \ldots\}$ for the given channel c of ρ_c, the transmission matrix (88) experiences exponential decay of $1/|H_+(\rho)|$ leading to the evanescence of the cross section (82) or (87). In effect, this means that the $|O_c(\rho_c)|$ term in Eq. (83) asymptotically acts like a Heaviside function, being unity for open channels, but closing the channels below threshold. Since $\rho_c = k_c r_c$ for the outgoing scattered wave $O_c(\rho_c)$, the exponential closure depends on two factors: the distance r_c from the nucleus and how far from the threshold one is $|E - E_{T_c}|$. This is a classical evanescence behavior of quantum tunneling.

What happens when continuing on the physical sheet $\{E, \ldots, +_c, \ldots\}$, as $|H_+(\rho)|$ will now tend to diverge as a "divide by zero"? The authors have no rigorous answer, but point to the fact that since E is left unchanged by the choice of the k_c sheet, the evanescence result ought to also stand, despite the apparent divergence.

Note that for photon channels, the semiclassic wave-number energy $\rho(E)$ mappings (3) of Sec. II.A of Ref. [22] do not yield this behavior; only the relativistic mapping (4) does. ■

We can estimate the orders of magnitude required to experimentally observe this evanescent quantum tunneling closure of the cross sections below threshold. At distance r_c from the center of mass of the nucleus, and at wave number k_c, distant from the threshold as $|E - E_{T_c}|$, the asymptotic behavior or the cross section below threshold is

$$\ln(\sigma_{cc'}(k_c, r_c)) \underset{k_c \to -\infty}{\overset{E_c \lesssim E_{T_c}}{\sim}} -2r_c|k_c|. \tag{91}$$

Assuming a detector is placed at a distance r_c of the nucleus, the cross section would decay exponentially below threshold as the distance $\Delta E_c = |E - E_{T_c}|$ of E to the threshold E_{T_c} increases. For instance, for a threshold of ^{238}U target reacting with neutron n channel, evanescence (91) would be of the rate of $\log_{10}(\sigma_{cc'}(k_c, r_c)) \sim -3 \times 10^{16} r_{\mathrm{cm}} \sqrt{\Delta E_{\mathrm{ceV}}}$. For a detector placed at a millimeter $r_c \approx 10^{-3}$ m, this means one order of magnitude is lost for the cross section in $\Delta E_c \approx 10^{-27}$ eV, evanescent indeed. Conversely, detecting this quantum tunneling with a detector sensitive to micro-electron volts $\Delta E_c \approx 10^{-6}$ eV ≈ 1 μeV (200 times more sensitive than the thermal energy of the cosmic microwave background) would see the cross section drop by one order of magnitude for a move of less than 10^{-13} m, or a tenth of a picometer. The quantum tunneling occurs at subatomic level: the outgoing wave disappears long before reaching the electron cloud.

Regardless of the evanescence of the transmission matrix, a more general argument on the cross section shows that analytic continuation of the above-threshold expressions will automatically close the channels below the threshold.

Theorem 6. ANALYTIC CONTINUATION ANNULS SUBTHRESHOLD CROSS SECTIONS.

For massive particles, analytic continuation of above-threshold cross-section expressions to complex wave numbers $k_c \in \mathbb{C}$ will automatically close channels for real energies $E \in \mathbb{R}$ below thresholds $E - E_{T_c} < 0$.

Proof. The proof is based on the fact that massive particles are subject to mappings (2) or (4) in Sec. II.A of Ref. [22], which entail wave numbers are real above threshold, and purely imaginary subthreshold: $\forall E < E_{T_c}, k_c \in \mathrm{i}\mathbb{R}$. Let $\psi(\vec{r})$ be a general wave function, so that the probability density is $|\psi|^2(\vec{r})$.

For a massive particle subject to a real potential, the de Broglie nonrelativistic Schrödinger equation applies, so that writing the conservation of probability on a control volume and applying the Green-Ostrogradsky theorem will yield the following expression for the probability current vector:

$$\vec{j}_\psi \triangleq \frac{\hbar}{\mu} \mathrm{Im}[\psi^* \vec{\nabla} \psi], \tag{92}$$

where μ is the reduced mass of the two-particle system [cf. Eqs. (2.10) and (2.12) in Sec. VIII.2.A, p. 312, in Ref. [1]). By definition, the differential cross section $\frac{d\sigma_{cc'}}{d\Omega}$ is the ratio

of the outgoing current in channel c' by the incoming current from channel c, by unit of solid angle $d\Omega$.

Consider the incoming channel c, classically modeled as a plane wave, $\psi_c(\vec{r}_c) \propto e^{i\vec{k}_c\cdot\vec{r}_c}$; and the outgoing channel c', classically modeled as radial wave, $\psi_{c'}(r_{c'}) \propto \frac{e^{ik_{c'}r_{c'}}}{r_{c'}}$. For arbitrary complex wave numbers, $k_c, k_{c'} \in \mathbb{C}$, Definition (92) will yield the following probability currents respectively:

$$\vec{j}_{\psi_c} \propto \frac{\hbar}{\mu}\mathrm{Im}[i\vec{k}_c e^{-2\mathrm{Im}[\vec{k}_c]\cdot\vec{r}_c}],$$
$$\vec{j}_{\psi_{c'}} \propto \frac{\hbar}{\mu}\mathrm{Im}\left[\left(ik_{c'} - \frac{1}{r_{c'}}\right)\frac{e^{-2\mathrm{Im}[k_{c'}]\cdot r_c}}{r_{c'}^2}\right]\vec{e}_r. \tag{93}$$

One will note these expressions are not the imaginary part of an analytic function in the wave number, because of the imaginary part $\mathrm{Im}[k_c]$. However, if we look at real wave numbers $k_c, k_{c'} \in \mathbb{R}$, that is, at above-threshold energies $E \geqslant E_{T_c}$, the probability currents (93) readily simplify to

$$\vec{j}_{\psi_c} \propto \frac{\hbar}{\mu}\mathrm{Re}[\vec{k}_c], \quad \vec{j}_{\psi_{c'}} \propto \frac{\hbar}{\mu}\mathrm{Re}[k_{c'}]\vec{e}_r. \tag{94}$$

These expressions are the real part of analytic functions of the wave numbers. If we analytically continue them to complex wave numbers and consider the cases of subthreshold reactions $E < E_{T_c}$ for either the incoming or the outgoing channel, the wave numbers are then exactly imaginary, $k_c, k_{c'} \in i\mathbb{R}$. The real parts in Eq. (94) become zero, thereby annulling the cross section $\sigma_{c,c'}(E)$. This means that for massive particles (not massless photons) subject to real potentials, analytic continuation of the probability currents expressions above threshold (94) will automatically close the subthreshold channels. This is true regardless of whether the transmission matrix (80) is or is not evanescent below threshold. This constitutes another major argument in favor of analytic continuation of open-channel expressions to describe the closed channels. ■

Note that for photon channels the derivations for the probability current vector (92) do not stand, and the wave number k_c is not imaginary below threshold using mapping (2) nor using the relativistic correction (4) of Sec. II.A of Ref. [22]. The fundamental reason why photon treatment is not straightforward is that R-matrix theory was constructed on the semiclassical formalism of quantum physics, with wave functions instead of state vectors. Though not incorrect, this wave-function approach of quantum mechanics does not translate directly for photons, though some work has been done to describe photons through wave functions [74,75]. This is another open area in the field of R-matrix theory, beyond the scope of this article.

V. CONCLUSION

In this article, we conduct a study and establish novel properties of the Siegert-Humblet pole expansion in radioactive states, which we show links R-matrix theory to the Humblet-Rosenfeld pole expansions of the scattering matrix. The Siegert-Humblet parameters are the poles $\{\mathcal{E}_j\}$ and residue widths $\{r_{j,c}\}$ of the Kapur-Peierls $\boldsymbol{R}_L$ operator (4). They are $N_L \geqslant N_\lambda$ complex and (almost always) simple poles that reside on the Riemann surface of mapping (1), composed of 2^{N_c} branches, for which one must specify on which sheet they reside, as shown in Theorem 1. They are intimately interwoven in that not any set of complex parameters is physically acceptable: They must be solution to (11). Both $\{\mathcal{E}_j\}$ and $\{r_{j,c}\}$ are invariant to changes in boundary conditions $\{B_c\}$. Furthermore, $\{\mathcal{E}_j\}$ is invariant to a change in channel radii $\{a_c\}$, and we established in Theorem 2 a simple way of transforming the radioactive widths $\{r_{j,c}\}$ under a change of channel radius a_c. Since the Siegert-Humblet parameters are the poles and residues of the local Mittag-Leffler expansion (10) of the Kapur-Peierls operator $\boldsymbol{R}_L$, the set of Siegert-Humblet parameters $\{E_{T_c}, a_c, \mathcal{E}_j, r_{i,c}\}$ is insufficient to entirely determine the energy behavior of the scattering matrix $\boldsymbol{U}$ through (42) and (41). The latter expressions directly link the R-matrix parameters to the poles and residues of the Humblet-Rosenfeld expansion of the scattering matrix and can be complemented by local coefficients $\{\boldsymbol{s}_n\}_{\mathcal{W}(E)}$ of the entire part (43) to untangle the energy dependence of the scattering matrix into a simple sum of poles and residues (41), which is the full Humblet-Rosenfeld expansion of the scattering matrix. Theorem 3 establishes that under analytic continuation of the R-matrix operators, the poles of the Kapur-Peierls $\boldsymbol{R}_L$ operator (i.e., the Siegert-Humblet radioactive poles) are exactly the poles of the scattering matrix $\boldsymbol{U}$.

The latter is one of three results we advance to argue that, contrary to the legacy force closure of subthreshold channels presented in Lane and Thomas [2], R-matrix operators ought to be analytically continued for complex momenta. Such analytic continuation is necessary to cancel the spurious poles which would otherwise be introduced by the outgoing wave functions, as we establish in Theorem 3. Moreover, we show in Theorem 4 that the analytic continuation of R-matrix operators in scattering matrix parametrization (2) enforces Eden and Taylor's generalized unitarity condition (70). Finally, we argue in Theorems 5 and 6 that analytic continuation will still close cross sections for massive particle channels (not massless photon channels) below threshold.

We thus conclude that the R-matrix community should henceforth come to consensus and agree to set the analytic continuation as the standard way of computing R-matrix operators [in particular, the shift $S_c(E)$ and penetration $P_c(E)$ functions] when performing nuclear data evaluations.

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