Scattering matrix pole expansions
&
invariance with respect to R-matrix parameters

Pablo Ducru∗ and Benoit Forget†
Massachusetts Institute of Technology
Department of Nuclear Science & Engineering
77 Massachusetts Avenue,
Cambridge, MA, 02139 U.S.A.

Vladimir Sobes‡
Oak Ridge National Laboratory
Directorate of Nuclear Science & Engineering
1 Bethel Valley Road, Oak Ridge, TN, 37831 U.S.A.

Gerald Hale§ and Mark Paris¶
Los Alamos National Laboratory
Theoretical Division (T-2)
MS B283, Los Alamos, NM 87545 U.S.A.

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A plethora of nuclear interactions have been modeled with R-matrix theory, upon which our current nuclear data libraries are based [1]. The R-matrix scattering model can parametrize the energy dependence of the scattering matrix in different ways. This article studies and establishes new results on three such sets of parameters — the Wigner-Eisenbud, the Brune, and the Siegert-Humblet parameters — showing how the latter two arise from the invariance of the scattering matrix to the Wigner-Eisenbud boundary condition $B_c$. We exhibit how these parametrizations strike an arbitrage between the complexity of their parameters, and the complexity of the energy dependence they entail for the scattering matrix. In this, our work bridges R-matrix theory with the well-known pole expansions of the scattering matrix developed by Humblet and Rosenfeld [2].

With respect to invariance to the channel radius $a_c$, we establish for the first time that the scattering matrix’s invariance to $a_c$ sets a partial differential equation on the widths of the Kapur-Peierls operator $R_L$. This enables us to derive an explicit transformation of the Siegert-Humblet radioactive residue widths $\{r_{j,c}\}$ under a change of channel radius $a_c$.

Considering the continuation of the scattering matrix to complex energies, several new results are established. We unveil there exist more Brune parameters than previously thought, depending on the way the scattering matrix is continued to complex energies. This points to a broader conundrum in the field: how to analytically continue the scattering matrix $U(E)$ while opening and closing channels at the threshold energies. On this question, we show that the legacy of Lane & Thomas to force-close channels below threshold – by defining the shift $S_c$ and penetration $P_c$ functions as the real and imaginary parts of the outgoing wave function reduced logarithmic derivative $L_c$ in order to annul elements of the scattering matrix $U_{cc}'$ below threshold – presents serious drawbacks when considering complex wavenumbers: this introduces nonphysical, spurious poles to the scattering matrix, while breaking its analytic properties. We show that the roots of the outgoing wave functions $O_c$ should introduce spurious poles to the scattering matrix, but that analytic continuation of the scattering matrix $U_{cc}'$ with constant Wronskian cancels them out. Moreover, we show that analytic continuation of R-matrix operators enforces the generalized unitarity conditions described by Eden & Taylor [3]. 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, and a physical argument based on the definition of the cross section as the ratio of probability currents.
I. INTRODUCTION

Myriad scattering phenomena in nuclear physics are modeled with R-matrix theory, with applications to nuclear simulation, radiation transport, astrophysics and cosmology, and extending to particle physics or atomistic and molecular simulation [4][5][6][7–11]. In essence, a scattering event 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). This partitioning, along with an orthogonality assumption of channels at the channel boundary, is what we could call the $R$-matrix scattering model, described by Kapur and Peierls in their seminal article [12], unified by Bloch in [13], and reviewed by Lane and Thomas in [5]. It is possible to study the general energy and wavenumber dependence of the scattering matrix emerging from this model, and such expansions were thoroughly studied by Humblet and Rosenfeld in [2, 14–21]. Alternatively, this wave-number dependence of the different possible outgoing particle-waves stemming from the R-matrix model can be parametrized, for calculability reasons, in several ways.

Over the years, different such parametrizations have been proposed for this same R-matrix model. The one that has come to prevail in the nuclear physics community is the Wigner-Eisenbud parametrization [5, 13, 22]. There are good reasons for this: the Wigner-Eisenbud parameters are unconstrained real parameters — i.e. though physically and statistically correlated, any set of real parameters is physically acceptable (though not necessarily likely nor present in nature) — that separate and parametrize the interior interaction Hamiltonian (usually an intractable many-body nuclear problem) from the exterior one (usually a well-known free-body or Coulomb Hamiltonian with analytic Harmonic expansions). Thus, Wigner and Eisenbud constructed a parametrization of the scattering matrix for calculability purposes: introducing simple real parameters that help de-correlate what happens in the inner interaction region from the asymptotic outer region.

But there exists other parametrizations of the R-matrix model, all with their advantages and disadvantages for interpretability or for subsequent treatment. In particular, we shall here focus on three such parametrizations: the Wigner-Eisenbud (which we will refer to as the $R_B$ for reasons that will become evident)[22]; the Brune (which we will henceforth refer to as $R_S$)[23]; and the Siegert-Humblet (henceforth $R_L$)[24, 25]. Since they all parametrize the wave-number dependence of the same R-matrix scattering model, these three parametric representations are physically equivalent, and one can go from one set of parameters to another through mathematical transformations we will hereafter explicit. For the same reasons, these parametrizations must also all be physically equivalent to the scattering matrix expansions of Humblet and Rosenfeld.

This article focuses on various properties of the Wigner–Eisenbud, Brune, and Siegert-Humblet respective parametrizations of the R-matrix model. We bring new insights to the invariance properties of the three different parametrizations and show that they entail a tradeoff between the complexity of the parameter space and the simplicity of the energy (or wave-number) dependence. Although invariance to the channel boundary condition $B_c$ has been well studied and is at the core of Brune’s alternative parametrization, we here unveil new properties of the Brune transform, in theorems 1, 2, and 3, as well as of the poles of the scattering matrix, invariant to the representation chosen. In this, we explicitly bridge the R-matrix parameters to the Humblet-Rosenfeld expansions of the scattering matrix, through equations (78) and (79). We also investigate invariance with respect to the channel radius $a_c$, which is a much less thoroughly explored topic in the literature, leading us to new insights with respect to the residues of the Siegert-Humblet $R_L$ parametrization, established in theorems 4 and 5. Finally, we argue, through theorems 6, 7, 8, 9, and 10, that contrary to what Lane & Thomas prescribed [5], the R-matrix parametrization should be analytically continued to complex wave-numbers $k_c \in \mathbb{C}$.

II. R-MATRIX WIGNER-EISENBDU PARAMETRIZATION

We here recall some fundamental definitions and equations of the Wigner-Eisenbud R-matrix parameters [5, 13, 22]. As described in Lane & Thomas, for each channel $c$, the two-body-in/two-body-out R-matrix model allows one to reduce the many-body system into a reduced one-body system. All the study is then performed in the reduced system and we consider the wave-number of each channel $k_c$, which we can render dimensionless using the channel radius $a_c$ and defining $\rho = \text{diag} (\rho_c)$ with $\rho_c = k_c a_c$.

A. Energy dependence and wavenumber mapping

All of the channel wavenumbers link back to one unique total system energy $E$, eigenvalue of the total Hamiltonian. Conservation of energy entails that this energy $E$ must be the total energy of any given channel $c$ (c.f. equation (5.12), p.557 of [2]):

$$E = E_c = E_{c'} = \ldots , \forall c$$  (1)

Each channel’s total energy $E_c$ is then linked to the wavenumber $k_c$ of the channel by its corresponding relation (6), say (4) and (5).
In the semi-classical model described in Lane & Thomas [5], we can separate on the one hand massive particles, for which the wavenumber $k_c$ is related to the center-of-mass energy $E_c$ of relative motion of channel $c$ particle pair with masses $m_{c,1}$ and $m_{c,2}$ as

$$k_c = \sqrt{\frac{2m_{c,1}m_{c,2}}{(m_{c,1} + m_{c,2})\hbar^2}} (E_c - E_{T_c})$$  \hspace{1cm} (2)$$

where $E_{T_c}$ denotes a threshold energy beyond which the channel $c$ is closed, as energy conservation cannot be respected ($E_{T_c} = 0$ for reactions without threshold). On the other hand, for a photon particle interacting with a massive body of mass $m_{c,1}$ the center-of-mass wavenumber $k_c$ is linked to the total center-of-mass energy $E_c$ of channel $c$ according to:

$$k_c = \frac{(E_c - E_{T_c})}{2\hbar c} \left[1 + \frac{m_{c,1}c^2}{(E_c - E_{T_c}) + m_{c,1}c^2}\right]$$  \hspace{1cm} (3)$$

Alternatively, in a more unified approach, one can perform a relativistic correction and smooth these differences away by means of the special relativity Mandelstam variable $s_c = (p_{c,1} + p_{c,2})$, also known as the square of the center-of-mass energy, where $p_{c,1}$ and $p_{c,2}$ are the Minkowsky metric four-momenta of the two bodies composing channel $c$, with respective masses $m_{c,1}$ and $m_{c,2}$ (null for photons). The channel wavenumber $k_c$ can then be expressed as:

$$k_c = \frac{\sqrt{s_c - (m_{c,1} + m_{c,2})^2 c^2}}{4\hbar c} \sqrt{s_c - (m_{c,1} - m_{c,2})^2 c^2}$$  \hspace{1cm} (4)$$

and the Mandelstam variable $s_c$ can be linked to the center-of-mass energy of the channel $E_c$ through

$$E_c = \frac{s_c - (m_{c,1} + m_{c,2})^2 c^2}{2(m_{c,1} + m_{c,2})}$$  \hspace{1cm} (5)$$

Interestingly, this is identical to the non-relativistic expression for the center-of-mass energy in terms of the lab energy in whichever channel the total mass $(m_{c,1} + m_{c,2})$ is chosen to be the reference for $E$ (but not in any other). This special relativistic correction to the non-relativistic R-matrix theory is the approach taken by the EDA code in use at the Los Alamos National Laboratory [26, 27].

Regardless of the approach taken to link the channel energy $E_c$ to the channel wavenumber $k_c$, conservation of energy (1) entails there exists a complex mapping linking the total center-of-mass energy $E$ to the wavenumbers $k_c$, or their associated dimensionless variable $\rho_c = k_c r_c$:

$$\rho_c(E) \leftrightarrow E$$  \hspace{1cm} (6)$$

Critical properties throughout this article will stem from the analytic continuation of R-matrix operators. As the outgoing $O_c$ and incoming $I_c$ wave functions are defined according to $\rho_c$ (c.f. section II.B below), the natural variable to perform analytic continuation is thus $\rho_c$, which is equivalent to extending the wavenumbers into the complex plane $k_c \in \mathbb{C}$. We can see that the mapping (6) from complex $k_c$ to complex energies is non-trivial, specially since the wavenumbers are themselves all interconnected. This creates a multi-sheeted Riemann surface, with branchpoints at each threshold $E_{T_c}$, well documented by Eden & Taylor [3] (also c.f. section 8 of [2]). More precisely, when calculating $\rho_c$ from $E$ one has to chose which sign to assign to $\pm \sqrt{E - E_{T_c}}$ in (2), or more generally to the mapping (4). Figure 1 shows this for the semi-classical case of massive particles (2), with zero threshold $E_{T_c} = 0$. Each channel $c$ thus introduces two choices, and hence there are $2^{N_c}$ sheets to the Riemann surface mapping (1) to (6), with the branch points close or equal to the threshold energies $E_{T_c}$. As we will see, the choice of the sheet will have an impact when finding different R-matrix parameters.

![Figure 1](image_url)  \hspace{1cm} FIG. 1. $\rho(E)$ mapping for massive particles in the semi-classical limit (2). The square root $\rho_c(E) = \pm \rho_0 \sqrt{E - E_{T_c}}$ gives rise to two sheets: $\{E, +\}$ and $\{E, -\}$.

### B. External region wave functions

In the R-matrix model, the external region is subject to either a Coulomb interaction or a free particle movement. In either case, the solutions form a two-dimensional vector space, a basis of which is composed of the incoming and outgoing wave functions: $O(k) := \text{diag} \{O_c(k_c)\}$, $I(k) := \text{diag} \{I_c(k_c)\}$. These are Whittaker or confluent hypergeometric function whose analytic continuation is discussed in section II.2.b and the appendix of [5], and for whose elemental properties and calculation we refer to chapter 14 of [28] and chapter 33 of [29], as well as Powell [30], Thompson [31], and Michel [32].

Note that the incoming and outgoing wave functions are only dependent on the wavenumber of the given channel $k_c$, this is a fundamental hypothesis of the R-matrix model. For clarity of writing, we will not explicitly write...
In lemma 1, we establish the Mittag-Leffler expansion of $L_c(\rho)$. Importantly, the Wronskian of the system is constant: 
\[ \forall \rho_c, \quad w_c = O_c^{(1)} I_c - I_c^{(1)} O_c, \] 
or with identity matrix $I$:
\[ w := O^{(1)} I - I^{(1)} O = 2i I. \]  

Of central importance to R-matrix theory is the Bloch operator, $\mathcal{L}$, which Claude Bloch introduced as the opérateur de conditions aux limites in equation (35) of [13], and that projects the system radially onto the channel boundaries for each channel, at the channel radius $r_c = a_c$. The Bloch operator $\mathcal{L}$ is then added to the Hamiltonian to form a compact Hermitian operator in the internal region (c.f. equation (34) of [13]), from which one can extract a complete discrete generative baseline of the Hilbert space. This is the essence of R-matrix theory, as best described by Claude Bloch in [13].

This projection on the channel boundaries at $r_c = a_c$, gives rise to the as yet unnamed quantity $L(\rho)$, introduced in equation (1.6a), section VII.1, p.289 of [5], and which can be recognized in equation (57) of [13], that is defined for each channel as:

\[ L_c^0(\rho_c) := L_c(\rho_c) - B_c \]  
where $\rho_c = k_\ell a_c$ has been projected on the channel surface, $B_c$ is the arbitrary outgoing-wave boundary condition, and $L_c(\rho_c)$ is the dimensionless reduced logarithmic derivative of the outgoing-wave function at the channel surface:

\[ L_c(\rho_c) := \frac{\rho_c \partial O_c}{O_c \partial \rho_c} \]  
or, equivalently, in matrix notation, and where $[\cdot]^{(1)}$ designates the derivative with respect to $\rho_c$:

\[ \mathbf{L} = \text{diag}(L_c) = \rho O^{-1} O^{(1)} \]  

so that the $L^0$ matrix function is written: $L^0 := \mathbf{L} - B$.

Using the Powell recurrence formulae [30], R.G. Thomas established the following scheme to calculate the outgoing-wave reduced logarithmic derivatives $L_\ell$ for different angular momenta $\ell$ values in the Coulomb case (c.f. p.350, appendix of [5], eqs.(A.12) and (A.13))

\[ L_\ell = \frac{a_\ell}{b_\ell - L_{\ell-1}} - b_\ell \]  

with

\[ a_\ell := \rho^2 + \left( \frac{\rho \eta}{\ell} \right)^2, \quad b_\ell := \ell + \left( \frac{\rho \eta}{\ell} \right) \]  

where $\eta = \frac{2\pi Z e^2 M_o a_c}{\hbar^2} \rho_c$ is the dimensionless Coulomb field parameter.

In general, both $O_c(\rho)$ and $L_c(\rho)$ are meromorphic functions of $\rho$ with a priori an infinity of poles, and for whose computation we refer to [30–32]. In lemma 1, we here establish the Mittag-Leffler expansion of $L_c(\rho)$.

**Lemma 1. Outgoing-wave reduced logarithmic derivative $L_c(\rho)$ Mittag-Leffler expansion.**

The outgoing-wave reduced logarithmic derivative $L_c(\rho)$, defined in (9), admits the following Mittag-Leffler pole expansion:

\[ \frac{L_c(\rho)}{\rho} = \frac{-\ell}{\rho} + i + \sum_{n \geq 1} \frac{1}{\rho - \omega_n} \]  

where $\{\omega_n\}$ are the roots of the outgoing wavefunctions $O_c(\rho)$. For neutral particles, there are a finite number of such roots, reported in table III.

**Proof.** From definition (9), $L_c$ is the reduced logarithmic derivative of the outgoing wavefunction $L_c(\rho) := \rho \frac{O_c^{(1)}(\rho)}{O_c(\rho)}$. In both the Coulomb and the neutral particle case, the outgoing wavefunction $O_c(\rho)$ is a confluent hypergeometric function with simple roots $\{\omega_n\}$. Moreover, their logarithmic derivative $\frac{O_c^{(1)}(\rho)}{O_c(\rho)}$ is bound at infinity. Thus, the following hypotheses stand:

- $L_\ell(\rho)$ has simple poles $\{\omega_n\}$, zeros of the $O_c(\rho)$,
- $L_\ell(\rho)$ has residues $\{\omega_n\}$ at the $\{\omega_n\}$ pole,
- $\exists M \in \mathbb{R}$ such that $|L_\ell(\rho)| < M |z|$ on circles $C_D$ as $D \to \infty$.

By removing the pole of $\frac{O_c^{(1)}(\rho)}{O_c(\rho)}$ at zero, these hypotheses ensure Mittag-Leffler expansion (14) to be verified:

\[ \frac{L_c(\rho)}{\rho} = L_\ell(0) + L_c^{(1)}(0) + \sum_{n \geq 1} \left[ \frac{1}{\rho - \omega_n} + \frac{1}{\omega_n} \right] \]  

R.G. Thomas’ recurrence formula (11) implies that $L_c(\rho_c)$ satisfies $L_\ell(0) = -\ell$, for both neutral and charged particles. Moreover, evaluating $\frac{O_c^{(1)}(\rho)}{O_c(\rho)}$ at the limit of infinity yields:

\[ L_c^{(1)}(0) + \sum_{k \geq 1} \frac{1}{\omega_k} = \lim_{\rho \to \infty} \left( \frac{L_c(\rho)}{\rho} \right) = \lim_{\rho \to \infty} \left( \frac{O_c^{(1)}(\rho)}{O_c(\rho)} \right) = i \]  

so that the Mittag-Leffler expansion (14) takes the desired form of (13).

Lemma 1 establishes the Mittag-Leffler expansion of $L_c^0(\rho_c)$ as a function of the roots $\{\omega_n\}$ of the outgoing wavefunctions $O_c(\rho)$, which are Hankel functions in the neutral particle case, and Whittaker functions in the more general case of charged particles (c.f. equations (2.14b) and (2.17) section III.2.b, p.269 of [5]). Extensive literature covers these functions [28, 29]. In the neutral particles case of Hankel functions [33–38] the search for their zeros established that the reduced logarithmic derivative of the outgoing wave function is a rational function of $k_\ell$ of degree $\ell$. In the general case there are indeed $\ell$ zeros to the Hankel function for $|\Re(\rho)| < \ell$, but for $|\Re(\rho)| > \ell$
TABLE I. Reduced logarithmic derivative \( L_\ell(\rho) := \frac{\partial \ln \rho}{\partial \rho} \) of outgoing wavefunction \( O_\ell(\rho) \), and \( L_\ell^0(\rho) := L_\ell(\rho) - B_\ell \) using \( B_\ell = -\ell \), irreducible forms and Mittag-Leffler pole expansions for neutral particles, for angular momenta \( 0 \leq \ell \leq 4 \).

| \( \ell \) | \( L_\ell(\rho) \) from recurrence (11) | \( L_\ell^0(\rho) \) using \( B_\ell = -\ell \) in (11) | \( L_\ell(\rho) \) from lemma 1, poles \( \{ \omega_n \} \) from table III | Outgoing wavefunction \( O_\ell(\rho) \) from (16) |
|---|---|---|---|---|
| 0 | \( \frac{1}{1+i\rho/\rho^2} \) | \( \frac{1+i\rho/\rho^2}{1-i\rho/\rho^2} \) | \( \{ 0 \} \) | \( e^{\rho} \) |
| 1 | \( \frac{1}{6+6i\rho^3-4i\rho^3} \) | \( \frac{1+i\rho/\rho^2}{3-3i\rho^2/\rho^2} \) | \( \omega_{1,2}^\ell = -i \) | \( e^{\rho} \left( \frac{1}{\nu} - 1 \right) \) |
| 2 | \( \frac{1}{-3+3i\rho^2+6i\rho^2} \) | \( \frac{1+i\rho/\rho^2}{3-3i\rho^2/\rho^2} \) | \( \omega_{3,4}^\ell \approx \pm 0.86602 - 1.5i \) | \( e^{\rho} \left( \frac{1}{\nu} - \frac{3}{\nu} - \frac{6}{\nu} + 1 \right) \) |
| 3 | \( \frac{1}{-45+45i\rho^2+60i\rho^2} \) | \( \frac{1+i\rho/\rho^2}{3-3i\rho^2/\rho^2} \) | \( \omega_{5,6}^\ell \approx \pm 2.32219i \) | \( e^{\rho} \left( \frac{1}{\nu} - \frac{1}{\nu} - \frac{6}{\nu} + i \right) \) |
| 4 | \( \frac{1}{-420+420i\rho^2+520i\rho^2+60i\rho^2+4i\rho} \) | \( \frac{1+i\rho/\rho^2}{3-3i\rho^2/\rho^2} \) | \( \omega_{7,8}^\ell \approx \pm 2.65736 - 2.10397i \) | \( e^{\rho} \left( \frac{1}{\nu} - \frac{1}{\nu} - \frac{6}{\nu} + i \right) \) |

Similarly, table III contains the algebraically solvable cases of up to \( \ell = 4 \), past which Neils Abel and Evariste Galois theorems do not guarantee solvability of \( \{ \omega_n \} \) by radicals (c.f. Abel-Ruffini theorem and Galois theory).

C. Internal region parameters

Projections upon the orthonormal basis formed by the eigenvectors of the Hamiltonian completed by the Bloch operator \( \mathcal{L} \) allow for the parametrization of the interaction Hamiltonian in the internal region by means of the Wigner-Eisenbud resonance parameters \[13\], composed of both the real resonance energies \( E_\gamma \in \mathbb{R} \), and the real resonance widths \( \gamma_{\lambda,c} \in \mathbb{R} \). From the latter, and using Brune’s notation \( c := \text{diag} \left( E_\gamma \right) \) and \( \gamma := \text{mat} \left( \gamma_{\lambda,c} \right) \), the Channel \( R \) matrix, \( R \), is defined as

\[
R := \sum_{\lambda=1}^{N_\lambda} \frac{\gamma_{\lambda,c} \gamma_{\lambda,c}^T}{E_\lambda - E} = \gamma^T (E - E)_{\text{inv}}^{-1} \gamma
\]  

and the Level \( A \) matrix, \( A \), is defined through its inverse:

\[
A^{-1} := E - E_{\text{inv}} - \gamma (L - B) \gamma^T
\]  

where \( B = \text{diag} \left( B_\ell \right) \) is the outgoing-wave boundary condition, which is arbitrary, constant (non-dependent on the wavenumber), and for which Bloch demonstrated that if it is real (i.e. \( B_\ell \in \mathbb{R} \)), then the Wigner-Eisenbud resonance parameters are also real \[13\]. From this, one can view the Wigner-Eisenbud parameters as the set of channel radii \( a_\ell \), boundary conditions \( B_\ell \), resonance widths \( \gamma_{\lambda,c} \), resonance energies \( E_{\lambda} \) and thresholds \( E_{T,\gamma} \). This set of parameters fully determine the energy (or wavenumber) dependence of the scattering matrix \( U \) through equation (19).

D. Scattering matrix

As explained by Claude Bloch, the genius of the \( R \)-matrix theory is that it can combine the internal region with the external region to simply express the resulting scattering matrix \( U \) (also called collision matrix, and often noted \( S \), though we here stick to the Lane & Thomas
scripture $U$ for the scattering matrix) as:

$$U = O^{-1}I + w\rho^{1/2}O^{-1} [R^{-1} + B - L]^{-1} O^{-1}\rho^{1/2}$$

$$= O^{-1}I + 2i\rho^{1/2}O^{-1} \gamma^T A\gamma O^{-1} \rho^{1/2}$$

$$= O^{-1}I + 2i\rho^{1/2}O^{-1} R_L O^{-1} \rho^{1/2}$$

(19)

The equivalence between these channel and level matrix expressions stems from the identity $[R^{-1} + B - L]^{-1} = \gamma^T A\gamma$ which defines the Kapur-Peirels operator, $R_L$:

$$R_L := [R^{-1} - L^0]^{-1} = [R^{-1} + B - L]^{-1}$$

(20)

The Kapur-Peirels operator $R_L$ will play a central role in this article and is thoroughly discussed in section III C. Identity (20) can be proved by means of the Woodbury identity:

$$[A + BD^{-1}C]^{-1} = A^{-1} - A^{-1}B [D + CA^{-1}B]^{-1} CA^{-1}$$

(21)

Indeed, the application of the Woodbury identity (21) to equality (20), with $A_{\text{Wood}} = R^{-1}, B_{\text{Wood}} = L^0,$ and $C_{\text{Wood}} = D_{\text{Wood}} = I$ yields

$$[R^{-1} - L^0]^{-1} = R + RL^0 [I - RL^0]^{-1} R$$

$$= \gamma^T (e - E\mathbb{I})^{-1} (e - E\mathbb{I})^{-1} \gamma L^0 \times$$

$$\left [ I - \gamma^T (e - E\mathbb{I})^{-1} \gamma L^0 \right ]^{-1} \gamma^T (e - E\mathbb{I})^{-1} \gamma$$

and then reversely applying the Woodbury identity with $A_{\text{Wood}} = (e - E\mathbb{I}), B_{\text{Wood}} = -\gamma L^0, C_{\text{Wood}} = \gamma^T,$ and $D_{\text{Wood}} = I$ one now recognizes

$$[R^{-1} - L^0]^{-1} = \gamma^T (e - E\mathbb{I})^2 - \gamma^T \gamma L^0 \gamma^T \gamma$$

Consider the multi-sheeted Riemann surface stemming from the analytic continuation of mapping (6), a truly remarkable and seldom noted property of the Wigner-Eisenbud theory and the Wigner-Eisenbud parameters $\{a_c, B_c, \gamma_{\lambda_c}, E_\lambda, E_{T_c}\}$, we here focus on the fact that the fundamental physical operator describing the scattering event is the scattering matrix $U$, and while the threshold energies $E_{T_c}$ are intrinsic physical properties of the system, all the other Wigner-Eisenbud parameters $a_c, B_c, \gamma_{\lambda_c},$ and $E_\lambda$ are interrelated and depend on arbitrary values of the channel radius $a_c$, or the boundary condition $B_c$. Though the channel radius $a_c$ can have some physical interpretation, this is not the case of the boundary condition $B_c$. This section explains how the search to remove the explicit dependence of the parameters on the arbitrary boundary condition $B_c$ has lead to both the Brune $R_B$ parameters and the Siegert-Humblet $R_L$ parameters.

### III. CONSEQUENCES OF INVARIANCE WITH RESPECT TO BOUNDARY CONDITION PARAMETERS.

Having recalled essential results from R-matrix theory and the Wigner-Eisenbud parameters $\{a_c, B_c, \gamma_{\lambda_c}, E_\lambda, E_{T_c}\}$, we here focus on the fact that the fundamental physical operator describing the scattering event is the scattering matrix $U$, and while the threshold energies $E_{T_c}$ are intrinsic physical properties of the system, all the other Wigner-Eisenbud parameters $a_c, B_c, \gamma_{\lambda_c},$ and $E_\lambda$ are interrelated and depend on arbitrary values of the channel radius $a_c$, or the boundary condition $B_c$. Though the channel radius $a_c$ can have some physical interpretation, this is not the case of the boundary condition $B_c$. This section explains how the search to remove the explicit dependence of the parameters on the arbitrary boundary condition $B_c$ has lead to both the Brune $R_B$ parameters and the Siegert-Humblet $R_L$ parameters.

#### A. Invariance to $B_c$

The dependence of the Wigner-Eisenbud parameters to the boundary condition $B_c$ can be made explicit by fixing the channel radius $a_c$ and performing a change of boundary condition $B \rightarrow B'$. This must entail a change in resonance parameters $E_\lambda \rightarrow E'_\lambda$ and $\gamma_{\lambda_c} \rightarrow \gamma'_{\lambda_c}$ which leaves the scattering matrix $U$ unchanged.

As described by Barker in [41], such change of variables can be performed by noticing that $e - \gamma (B' - B) \gamma^T$ is a real symmetric matrix when both $B$ and $B'$ are real. The spectral theorem thus assures there exists a real orthogonal matrix $K$ and a real diagonal matrix $D$ such that

$$e - \gamma (B' - B) \gamma^T = K^T DK$$

(22)

The new parameters are then defined as

$$e' := D , \quad \gamma' := K\gamma$$

(23)

This change of variables satisfies:

$$\gamma'^T A_{B'} \gamma' = \gamma^T A_B \gamma$$

(24)

and thus leaves the scattering matrix unaltered through equation (19). Here $A_{B'}$ designates the level matrix from parameters $e', \gamma'$ and $B'$. Equivalently, using the Woodbury identity (21) shows that this change of variables verifies (c.f. eq.(4) of [41] or eq. (3.27) of [42]):

$$R^{-1}_{B'} + B = R^{-1}_B + B'$$

(25)

If the change of variable is infinitesimal, this invariance property translates into the following equivalent differential equations on the Wigner-Eisenbud $R_B$ matrix,

$$\frac{\partial R^{-1}_B}{\partial B} + I = 0 \quad \text{i.e.} \quad \frac{\partial R_B}{\partial B} - R^{-1}_B = 0$$

(26)
(c.f. eq (2.5b) section IV.2, p.274 of [5]) where we made use of the following property to prove the equivalence:

\[
\frac{\partial M^{-1}}{\partial z}(z) = -M^{-1}(z) \left( \frac{\partial M}{\partial z}(z) \right) M^{-1}(z)
\] (27)

B. Real invariant \( R_S \) parameters: Brune’s alternative parametrization

Since the physics of the system are invariant with the choice of the arbitrary \( B \), boundary condition, Brune built on Barker’s work [41] to propose an alternative parametrization of R-matrix theory in which the alternative parameters, \( \tilde{e} \) and \( \tilde{\gamma} \), are boundary-condition independent [23].

1. Definition of Brune’s \( R_S \) parametrization

Key to Brune’s alternative parametrization is the splitting of the outgoing-wave reduced logarithmic derivative – and thus the \( L^0 \) matrix function – into real and imaginary parts, respectively the shift \( S \) and penetration \( P \) factors:

\[
L = S + iP
\] (28)

From there, and with slight changes from the notation in [23], the physical level matrix \( \tilde{A} \) is defined as:

\[
\tilde{A}^{-1}(E) = \tilde{G} + \tilde{e} - E \left[ I + \tilde{H} \right] - \tilde{\gamma} L(E) \tilde{\gamma}^T
\] (29)

with

\[
\tilde{G}_{\lambda\mu} = \frac{\gamma_{\mu} (S_\mu \tilde{E}_\lambda - S_\lambda \tilde{E}_\mu)}{\tilde{E}_\lambda - \tilde{E}_\mu}
\] (30)

and

\[
\tilde{H}_{\lambda\mu} = \frac{\gamma_{\mu} (S_\mu - S_\lambda)}{\tilde{E}_\lambda - \tilde{E}_\mu}
\] (31)

such that with the new alternative resonance parameters, \( \tilde{E}_i \) and \( \tilde{\gamma}_{i,e,c} \), the following equality stands,

\[
\gamma^T A \gamma = \tilde{\gamma}^T A \tilde{\gamma}
\] (32)

and thus the scattering matrix \( U \) is left unchanged.

These alternative Brune parameters \( \tilde{e} \) and \( \tilde{\gamma} \) are no longer \( B \) dependent since the arbitrary boundary condition does not appear in the definition of the physical level matrix, and from there in the parametrization of the scattering matrix.

Brune explains how to compute his parameters from the Wigner-Eisenbud ones by finding the \( \{ \tilde{E}_i \} \) scalars and \( \{ g_i \} \) vectors (noted \( \{ a_i \} \) in [23]) that solve the generalized eigenproblem [23]:

\[
e - \gamma (S(E_i) - B) \gamma^T g_i = \tilde{E}_i g_i
\] (33)

and defining the Brune parameters as:

\[
\tilde{e} := \text{diag}(\tilde{E}_i), \quad \tilde{\gamma} := g^T \gamma
\] (34)

where \( g \) is the matrix composed of the column eigenvectors: \( g := [g_1, \ldots, g_i, \ldots] \). The physical level matrix is then defined as (c.f. equation (30), [23]):

\[
\tilde{A}^{-1} := g \tilde{A} g^T
\] (35)

which guarantees

\[
A := g \tilde{A} g^T
\] (36)

and thus (32), and whose explicit expression is (29).

Note that searching for the general eigenvalues in (33) is equivalent to solving (apply the Sylvester determinant identity theorem, or c.f. eq. (49)-(50) in [23]):

\[
\det (R_S^{-1}(E)) \bigg|_{E=E_i} = 0
\] (37)

i.e. solving for the poles of the \( R_S \) operator defined as

\[
R_S^{-1} := R^{-1} + B - S
\] (38)

hence our dubbing of the Brune parametrization as the \( R_S \) parametrization. We here provide additional insights into this alternative \( R_S \) parametrization of the R-matrix scattering model, which will be foretelling of the structure of the \( R_L \) parametrization discussed in section III.C.

The key insight is that in equation (22) of [23], Brune builds a square matrix \( g := [g_1, \ldots, g_i, \ldots] \), from which he is able to build the inverse physical level matrix in his equation (30) of [23]. Brune justifies that this matrix is indeed square in the paragraphs between equations (46) and (47) by a three-step monotony argument depicted in FIG. 1 of [23]: 1) he assumes \( S(E) \) is continuous (i.e. has no real poles); 2) he assumes \( \frac{\partial E}{\partial \beta} \geq 0 \), which is always true for negative energies and was just proved to be true for positive energies in the case of repulsive Coulomb interactions [43] (a general proof is lacking for positive energy attractive Coulomb channels but has always been verified in practice); 3) he invokes the eigenvalue repulsion behavior (no-crossing rule) of which these three assumption are true, since the left-hand-side of (33) is a real symmetric matrix for any real energy value, then the spectral theorem guarantees there exists \( N_\lambda \) real eigenvalues to it, and Brune’s three assumptions above elegantly guarantee that there exists exactly \( N_\lambda \) real solutions to the generalized eigenvalue problem (33).
2. Ambiguity in shift and penetration factors definition for complex wavenumbers

There is a subtlety, however. A careful analysis reveals that the assumption that $S_c(E)$ is continuous or monotonously increasing is not unequivocal, and points to an open discussion in the field of nuclear cross section evaluations: the way of continuing the scattering matrix $U$ to complex wavenumbers $k_c \in \mathbb{C}$. Indeed, there is an ambiguity in the definition of the shift $S_c(E)$ and penetration $P_c(E)$ functions: two approaches are possible, and the community is not clear on which is correct.

The first, Lane & Thomas approach is to define the shift and penetration functions as the real and imaginary parts of the two-outgoing-wave reduced logarithmic derivative:

$$
\forall E \in \mathbb{C}, \left\{ \begin{array}{l}
S(E) := \Re \left[ L(E) \right] \in \mathbb{R} \\
P(E) := \Im \left[ L(E) \right] \in \mathbb{R}
\end{array} \right. \quad (39)
$$

This definition, introduced in [5] III.4.a. from equations (4.4) to (4.7c), finds its justification in the discussion between equations (2.1) and (2.2) of [5] VII.2, as it presents the advantage of automatically closing the sub-threshold channels since:

$$
\forall E < E_{T_c}, \quad \exists [L_c(E)] = 0 \quad (40)
$$

This elegant closure of channels comes at two costs: 1) the scattering matrix $U$ is no longer analytic for complex wavenumbers $k_c \in \mathbb{C}$; 2) artificial poles are introduced to the scattering matrix, as we will show in theorem 6 that analytic continuation of $O$ and $I$ — and thus the operators $L$, $S$, and $P$ — is necessary to cancel the poles of $O$ out of the scattering matrix $U$. In this Lane & Thomas approach (39), the function calculated for $S$ changes from $S(E) := S_c(E)$ above threshold ($E \geq E_{T_c}$), to $S(E) := L_c(E)$ below threshold ($E < E_{T_c}$), because of (40). Moreover, definition (39) induces ramifications for both the shift and the penetration factors, as we show in lemma 2.

**Lemma 2. Branch-point definition of shift $S_c(E)$ and penetration $P_c(E)$ functions.**

**Definition (39)** of the shift $S_c(E)$ and penetration $P_c(E)$ functions, legacy of Lane & Thomas, entails:

- branch-points for both $S_c(E)$ and $P_c(E)$, induced by the multi-sheeted nature of mapping (6),
- on the $\{E, -\}$ sheet below threshold $E < E_{T_c}$, the shift function $S_c(E)$ can present discontinuities and areas where $\frac{\partial S}{\partial E}(E) < 0$,
- in particular, for neutral particles of odd angular momenta $\ell_c \equiv 1$ (mod 2), there is exactly one real sub-threshold pole to $S_c(E)$ on the $\{E, -\}$ sheet,
- everywhere other than sub-threshold $\{E, -\}$ sheet, and in particular on the $\{E, +\}$ sheet, the shift function $S_c(E)$ is continuous and monotonously increasing: $\frac{\partial S}{\partial E}(E) \geq 0$.

**Proof.** The proof simply introduces the branch-structure of the $\rho_c(E)$ mapping (6), observable in figure 1, into the Lane & Thomas definition (39). Historically, the study of the properties emanating from this definition have neglected the $\{E, -\}$ sheet. Importantly, it was recently proved that $\frac{\partial S_c(E)}{\partial E}(E) \geq 0$ was true for most cases [43].

This proof did not consider the $\{E, +\}$ sheet of mapping (6). However, their proof of $\frac{\partial S_c(E)}{\partial E}(E) \geq 0$ should still stand on the $\{E, +\}$ sheet. Moreover, the proof of lemma 3 establishes that all the discontinuity points, i.e. the real-energy poles, happen at sub-threshold energies, and in particular that neutral particles with odd angular momenta introduce exactly one such sub-threshold discontinuity. This means that above threshold, both the shift $S_c(E)$ and penetration $P_c(E)$ functions are continuous. These behaviors are depicted in figure 2. Finally, one will notice that the $\{E, +\}$ and $\{E, -\}$ sheets coincide above threshold for the shift function $S_c(E)$, and below threshold for the penetration function $P_c(E)$. For $P_c(E)$, this is because of property (40). For $S_c(E)$, this is because for real energies above threshold, both definitions (39) and (42) coincide, and lemma 3 shows the analytic continuation definition of $S_c(E)$ is function of $\rho_2^c(E)$, which unfolds the sheets of the Riemann mapping (6). Hence, for above-threshold energies, this property still stands for the Lane & Thomas definition of the shift factor $S_c(E)$. \hfill $\square$

The second approach to defining the shift and penetration functions, $S$ and $P$, consists of performing analytic continuation of the scattering matrix $U$ to complex energies $E \in \mathbb{C}$. This is implicit in the Kapur-Peirls or Siegert-Humblet expansions (c.f. section III.C), and an abundant literature revolves around the analytic properties of the scattering matrix in the complex plane, including the vast Theory of Nuclear Reaction of Humblet and Rosenfeld [2, 14–21], or the general unitarity condition on the multi-sheeted Riemann surface introduced by Eden and Taylor in [3]. In this approach, energy dependence of the shift and penetration factors for positive energies are analytically continued into the complex plane, i.e.

$$
S : \mathbb{C} \mapsto \mathbb{C} \quad \forall E \rightarrow S_c(E) \quad \text{s.t.} \quad S(E) = S_c(E), \forall (E - E_{T_c}) \in \mathbb{R}_{+} \quad (41)
$$

so that they can be computed from the outgoing wave-function reduced logarithmic derivative $L$ by analytic continuation in wavenumber space $k_c \in \mathbb{C}$:

$$
\forall \rho_c \in \mathbb{C}, \left\{ \begin{array}{l}
S_c(\rho_c) := L_{c}(\rho_c) + \left[ L_{c}(\rho_c^*) \right]^* \\
P_c(\rho_c) := \frac{L_{c}(\rho_c) - \left[ L_{c}(\rho_c^*) \right]^*}{2i} \in \mathbb{C}
\end{array} \right. \quad (42)
$$

From this definition (42), and using the recurrence relation (11), one readily finds the expressions for the neutral particles shift and penetration factors documented in table II. Critically, both definitions (39) and (42) will yield the same shift $S_c(E)$ and penetration $P_c(E)$ functions for real energies above threshold $E \geq E_{T_c}$. Moreover, definition (42) bestows interesting analytic properties onto
the shift and penetration functions, here established in lemma 3.

Lemma 3. Analytic continuation definition of shift \( S_c(E) \) and penetration \( P_c(E) \) functions. When defined by analytic continuation (42), the shift function, \( S_c(\rho) \), satisfies the Mittag-Leffler expansion:

\[
S_c(\rho) = -\ell + \sum_{n \geq 1} \frac{\rho^2}{\rho^2 - \omega_n^2} + \frac{\rho^2}{\rho^2 - \omega_n^*} \quad \text{arg}(\omega_n) \in [-\pi, 0]
\]

where the poles \( \{\omega_n\} \) are only the lower-right-quadrant roots - i.e. such that \( \text{arg}(\omega_n) \in [-\pi, 0] \) - of the outgoing wave function \( O_c(\rho) \). In the neutral particles cases, these are reported in table III. Given \( \rho_c(E) \) mapping (6), this entails \( S_c(E) \):

- unfolds the sheets of \( \rho_c(E) \) mapping (6),
- is purely real for real energies: \( \forall E \in \mathbb{R}, S_c(E) \in \mathbb{R} \).

The penetration function, \( P_c(\rho) \), satisfies the Mittag-Leffler expansion:

\[
P_c(\rho) = \rho \left[ 1 - i \sum_{n \geq 1} \frac{\omega_n}{\rho^2 - \omega_n^2} - \frac{\omega_n^*}{\rho^2 - \omega_n^*} \right]
\]

which in turn entails that \( P_c(E) \):

- is purely real for above threshold energies: \( \forall E > E_{T_c}, P_c(E) \in \mathbb{R} \),
- is purely imaginary for sub-threshold energies: \( \forall E < E_{T_c}, P_c(E) \in \mathbb{iR} \).

In the neutral particles case, Mittag-Leffler expansions (43) and (44) are the partial fraction decompositions of the rational fractions reported in table II, and for all odd angular momenta \( \ell_c \equiv 1 (\mod 2) \), both have one, shared, real sub-threshold pole.

Proof. The proof uses lemma 1, where we establish the Mittag-Leffler expansion (14) of the reduced logarithmic derivative \( L_c(\rho_c) \). Using the conjugacy properties (108) on the poles \( \{\omega_n\} \) means each pole \( \omega_n \) on the lower right quadrant of the complex plane - i.e. such that \( \text{arg}(\omega_n) \in [-\pi, 0] \) - induces a specular pole \( -\omega_n^* \). Dividing the poles in specular pairs, we can re-write the Mittag-Leffler expansion (14) as:

\[
L_c(\rho) = -\ell + i\rho + \sum_{n \geq 1} \frac{\rho}{\rho - \omega_n} + \frac{\rho}{\rho + \omega_n^*}
\]

Plugging-in expression (45) into the shift function definition (42) readily yields (43) and (44).

Note that (43) unfolds the Riemann surface of mapping (6), whereas (44) factors-out the branch points so that all its branches are symmetric. In (44) we recognize the odd powers of \( \rho \) in the neutral particles case of table II, which do not unfold the Riemann sheets of mapping (6). These behaviors are illustrated in figure 3.

In the neutral particles case, \( L_c \) is a rational fraction in \( \rho_c \), and its denominator is of degree \( \ell_c \), as can be observed in table I, thus inducing \( \ell_c \) poles, reported in table III. Since these poles \( \{\omega_n\} \) must respect the specular symmetry: \( \omega \leftrightarrow -\omega_n^* \), it entails that these poles come in symmetric pairs. For neutral particles, odd angular momenta mean there is an odd number of poles \( \{\omega_n\} \). For them to come in pairs thus imposes one is exactly imaginary \( \omega_n = -ix_n \), with \( x_n \in \mathbb{R}^+ \). When squared, this purely imaginary pole will introduce a purely sub-threshold pole in both (43) and (44), though: \( \frac{1}{\rho^2 + x_n^2} \).

An example to illustrate the difference between definitions (39) and (42) is depicted in figures 2 and 3. Consider the elemental case of a neutron channel with angular momentum \( \ell_c = 1 \), and let \( \rho_0 \) be the proportionality
TABLE II. Shift $S\ell\rho, S\ell\rho := S\ell\rho - B\ell$ using $B\ell = -\ell$, and $P\ell\rho$ irreducible forms for neutral particles, for angular momenta $0 \leq \ell \leq 4$, all defined from analytic continuation (42).

| $\ell$ | $S\ell\rho$ | $S\ell\rho$ := $S\ell\rho - B\ell$ (recurrence for $B\ell = -\ell$) | $P\ell\rho$ |
|-------|-------------|-------------------------------------------------|--------|
| 0     | 0           | $\rho^{2}((\ell - N_{s}c\rho)^{2} + p_{\ell-1}^{2}) - \ell$ | $\rho$ |
| 1     | $-\frac{1}{1 + \rho^{2}}\rho^{2}$ | $\frac{1}{1 + \rho^{2}}\rho^{2}$ | $\frac{1}{1 + \rho^{2}}\rho^{2}$ |
| 2     | $-\frac{1}{1 + \rho^{2}}\rho^{2}$ | $\frac{1}{1 + \rho^{2}}\rho^{2}$ | $\frac{1}{1 + \rho^{2}}\rho^{2}$ |
| 3     | $-\frac{675 + 90\rho^{2} + 6\rho^{4}}{225 + 45\rho^{2} + 6\rho^{4} + \rho^{6}}$ | $\frac{225 + 45\rho^{2} + 6\rho^{4} + \rho^{6}}{\rho^{2}}$ | $\frac{225 + 45\rho^{2} + 6\rho^{4} + \rho^{6}}{\rho^{2}}$ |
| 4     | $-\frac{44100 + 4725\rho^{2} + 2770\rho^{4} + 10\rho^{6}}{11025 + 1575\rho^{2} + 435\rho^{4} + 10\rho^{6} + \rho^{8}}$ | $\frac{11025 + 1575\rho^{2} + 435\rho^{4} + 10\rho^{6} + \rho^{8}}{\rho^{2}}$ | $\frac{11025 + 1575\rho^{2} + 435\rho^{4} + 10\rho^{6} + \rho^{8}}{\rho^{2}}$ |

\[S\ell\rho := S\ell\rho + \ell = \frac{\rho^{2}((\ell - N_{s}c\rho)^{2} + p_{\ell-1}^{2})}{(\ell - S\ell_{-1}(\rho))^{2} + p_{\ell-1}^{2}}\]

\[P\ell\rho := \frac{\rho^{2}((\ell - N_{s}c\rho)^{2} + p_{\ell-1}^{2})}{(\ell - S\ell_{-1}(\rho))^{2} + p_{\ell-1}^{2}}\]

constant so that (2) is written $\rho(E) = \pm \rho_{0}\sqrt{E - E_{T\rho}}$. Let us also set a zero threshold $E_{T\rho} = 0$, for simplicity.

In this case, the legacy Lane & Thomas definition (39) corresponds to taking $S(E) := S_{\ell}(\rho_{c}(E)) = -\frac{1}{1 + \rho^{2}}$ for above-threshold energies $E \geq E_{T\rho}$, and switch to $S(E) := L_{\ell}(\rho_{c}(E)) = \frac{1 + \rho^{2}}{1 + \rho^{2}}$ for sub-threshold energies $E < E_{T\rho}$. Since the (2) mapping $\rho(E) = \pm \rho_{0}\sqrt{E - E_{T\rho}}$ has two sheets, this means definition (39) entails: $S(E) := S_{\ell}(E) = -\frac{1}{1 + \rho_{c}^{2}}$ for $E \geq E_{T\rho}$, and $S(E) := L_{\ell}(E) = \frac{-1 + \rho_{c}^{2}\sqrt{E + \rho_{c}^{2}E}}{1 + \rho_{c}^{2}\sqrt{E + \rho_{c}^{2}E}}$ for $E < E_{T\rho}$, which is a real quantity. Definition (39) thus introduces the ramifications reported in figure 2. In particular, the full cyan line of our $\Re[L_{\ell}(E)]$ plot corresponds to the uncharged case for angular momentum $\ell = 0$ reported as a black curve in FIG.1, p.6 of [43]. Notice that all the $\{E, +\}$ curves are continuous and monotonically increasing ($\frac{\partial S}{\partial E} \geq 0$), which is in accordance to the monotonic properties established in [43]. However, on the $\{E, -\}$ sheet below threshold, $\Re[L_{\ell}(E)]$ is no longer monotonic for even angular momenta ($\frac{\partial \Re[L_{\ell}(E)]}{\partial E} \geq 0$ does not hold), and is discontinuous in the case of odd angular momenta.

In contrast, for our same elemental case, the analytic continuation definition (42) simply defines $S(E) := S_{\ell}(\rho_{c}(E)) = -\frac{1}{1 + \rho^{2}}$ for all real or complex energies $E \in \mathbb{C}$, that is $S(E) := -\frac{1}{1 + \rho_{c}^{2}}E$. The later happens to have a real pole, which introduces a discontinuity, at $E_{\text{dis}} = -\frac{1}{\rho_{c}^{2}}$, as can be seen in figure 3. One can observe that all odd angular momenta are monotonous but have a real sub-threshold pole. For even angular momenta, $S_{\ell}(E)$ is continuous, monotonically increasing above-threshold, but $\frac{\partial S}{\partial E}(E) \geq 0$ does not hold below-threshold. For the penetration function $P_{\ell}(E)$, each ramification is monotonous, but in opposite, mirror direction. In figure 3, the shift function $S_{\ell}(E)$ does not present branch points, as proved in lemma 3: it is a function of $\rho^{2}$ so no $\pm \sqrt{\rho}$ choice is necessary in $\rho_{c}(E)$ mapping (4).

3. Number of Brune poles

Definitions (39) and (41) have a major impact on the Brune parameters (34): they command that the number $N_{S}$ of Brune poles $\{\tilde{E}_{\ell}\}$, solutions to Brune’s generalized eigenproblem (33), is greater than the $N_{\lambda}$ previously found in [23]: i.e. $N_{S} \geq N_{\lambda}$. And this is regardless of whether definition (39) or (41) is chosen for the shift factor $S_{\ell}(E)$ when searching for these solutions.

The fundamental reason for this is that Brune’s three-step monotony argument, which elegantly proved in [23] that there are exactly $N_{\lambda}$ solutions to (33) and which we here recall in the last paragraph of section III B 1, rests on two hypotheses on the shift function $S_{\ell}(E)$: 1) it is continuous (i.e. has no real poles), and 2) it is monotonously increasing, i.e. $\frac{\partial S}{\partial E} \geq 0$. In [43], these two hypotheses have just been proved to hold true for energies above threshold $E \geq E_{T\rho}$, i.e. for real wavenumbers $k_{c} \in \mathbb{R}$. Yet, we just established in lemmas 2 and 3 that proper accounting of the multi-sheeted nature of the Riemann surface created by mapping (6) shows these two hypotheses do not hold for sub-threshold energies $E < E_{T\rho}$, where the wavenumber is purely imaginary from mapping (2). This engenders additional solutions to Brune’s generalized eigenproblem (33), so that the number $N_{S}$ of Brune poles $\{\tilde{E}_{\ell}\}$ is in fact greater than the number of channels: $N_{S} \geq N_{\lambda}$. So how many $N_{S}$ solutions are there? This depends on the R-matrix parameters and on the definition chosen for the shift function $S_{\ell}(E)$, as we now show in theorems 1 and 2, for definitions (39) and (41), respectively.

**Theorem 1.** Shadow Brune Poles.

Let the branch Brune poles $\{\tilde{E}_{\ell}\}$ be the solutions of the Brune generalized eigenproblem (33), using the legacy Lane & Thomas definition (39) for the shift $S_{\ell}(E)$, and let $N_{S}$ be the number of such solutions, then:

- all the branch Brune poles are real, and live on the $2N_{c}$ sheets of the Riemann surface from (6) mapping:

\[\tilde{E}_{1}, \ldots, \tilde{E}_{N_{c}} \in \mathbb{R}^{N_{c}}\]
FIG. 3. Shift $S_c(E)$ and penetration $P_c(E)$ functions for massive neutral particles, as defined by analytic continuation (42), for different angular momenta $\ell_c \in [0, 4]$. This definition induces no branch points for the shift function $S_c(E)$, as it unfolds the sheets of mapping (6), in this non-relativistic massive particles case (2), as shown in lemma 3. One can observe discontinuities (for odd angular momenta) and non-monotonic behavior (for even angular momenta) for sub-threshold energies. $P_c(E)$ is purely real, with branches, above threshold; and purely imaginary, with branches, below threshold.

- exactly $N_\lambda$ branch Brune poles are present on the $\{E, +, \ldots, +\}$ sheet of mapping (6), $N_\lambda$

- additional shadow Brune poles can be found below threshold, $E < E_{T_r}$, on the $\{E, -\}$ sheets of mapping (6), depending on the values of the resonance parameters $\{E_\lambda, \gamma_{\lambda c}, B_c, E_{T_r}, a_c\}$ – though in a way that is invariant under boundary-condition $B_c$

- each neutral particle, odd angular momentum $\ell_c \equiv 1 \pmod{2}$, channel adds at least one shadow Brune pole below threshold on its $\{E, -\}$ sheet, so that the total number $N_S^\pm$ of branch Brune poles on all sheets of mapping (6) is greater than the number $N_\lambda$ of levels: $N_S^\pm \geq N_\lambda$.

Proof. Let us go about solving the Brune generalized eigenproblem (33), following the three-step argument of Brune (c.f. last paragraph of section III B 1). We consider the left-hand side of (33). According to definition (39), the shift function is always real, even for complex wavenumbers $k_c \in \mathbb{C}$. Since by construction the Wigner-Eisenbud R-matrix parameters $\{E_\lambda, \gamma_{\lambda c}, B_c, E_{T_r}, a_c\}$ are also all real, this implies the right-hand side must be real to solve (33). Thus, all branch Brune poles from definition (39) are real. To find them, we follow Brune’s approach: for any energy $E$, on any of the $2^N_c$ sheets of mapping (6), the left-hand side is a real symmetric matrix, and its eigenvalue decomposition will thus yield $N_\lambda$ real eigenvalues: $\{\tilde{E}_i(E)\} \in \mathbb{R}$. We then have to vary the $E$ value until these real eigenvalues cross the $E = E$ identity line in the right-hand side. In general, the full accounting of all the Riemann sheets from mapping (6) will entail solutions of the generalized Brune eigenproblem (33) on all sheets. These branch Brune poles should thus be reported with the choice of sheet from the mapping (6) for each channel, as in (75) for the poles of the Kapur-Peierls operator of section III C 3: $\{\tilde{E}_i, +, - , \ldots, +\}$.

We state in lemma 2 than on the $\{E, +\}$ sheet, $S_c(E)$ is indeed continuous and monotonously increasing. We can thus apply Brune’s three-step argument: the $N_\lambda$ eigenvalues of the left-hand side of (33) will satisfy $\frac{\partial \tilde{E}_i(E)}{\partial E} \leq 0$, and thus each and every one of them will eventually cross the $E = E$ identity line exactly once as $E$ varies continuously. On the $\{E, +\}$ sheet for all channels, there are thus exactly $N_\lambda$ Brune poles: $\{\tilde{E}_i, +, - , \ldots, +\} \in \mathbb{R}^{N_\lambda}$

However, we showed in lemma 2 that $S_c(E)$ is not monotonous and can be discontinuous for sub-threshold energies $E < E_{T_r}$ on the $\{E, -\}$ sheet. So how many Brune poles are there on all sheets? Unfortunately, the number of solutions to Brune’s generalized eigenproblem
(33) will depend on the values of the resonance parameters \( \{ E_\lambda, \gamma_\lambda, B_c, E_{T}, a_c \} \) — though in a way that is invariant under change of boundary-condition \( B_c \), as made evident in (37) when considering invariance (25). That the number of solutions to (33) depends on the parameters can be observed in figure 5.

For neutral particles odd momenta \( \ell_c \equiv 1 \pmod{2} \) channels, lemma 2 also showed there exist exactly one sub-threshold pole to \( S_c(E) \) on the \( \{ E, - \} \) sheet of mapping (6). This pole will automatically cross the \( E = E \) line of Brune’s three-step argument twice, once below and once above threshold, adding an additional shadow Brune pole to the \( N_\lambda \) Brune found in [23]. This proves that there exists shadow Brune poles, just as shadow poles in the Siegert-Humblet parameters were revealed by G.Hale in [44, 45]. This behavior is illustrated in figure 4.

Theorem 1 establishes the existence of sub-threshold shadow Brune poles when the legacy Lane & Thomas definition (39) is chosen for the shift function \( S_c(E) \). If instead the analytic continuation definition (41) is chosen, we now show in theorem 2 that this unfolds the Riemann surface for the shift function \( S_c(E) \) so that no branch points are required to define the Brune parameters. In contrast, a drawback of definition (42) is that branch points are required to define the Brune parameters. In particular, we present an argument that analytic continuation can be used to define the Brune parameters.

Theorem 2.

Analytic Brune Poles.
Let the analytic Brune poles \( \{ \tilde{E}_i \} \) be the solutions of the Brune generalized eigenproblem (33), using the analytic continuation definition (42) for the shift \( S_c(E) \), and let \( N_S \) be the number of such solutions, then:

- the analytic Brune poles are in general complex, and live on the single sheet of the unfolded Riemann surface from (6) mapping: \( \tilde{E}_i \in \mathbb{C}^{N_S} \),

- in the neutral particle case, there are exactly \( N_S \) complex analytic Brune poles with:

\[
N_S = N_\lambda + \sum_{\ell_c = 1}^{N_c} \ell_c
\]

so that the number \( N_S \) of complex and \( N_S^R \) of real analytic Brune poles, \( \{ \tilde{E}_i \} \in \mathbb{R}^{N_S^R} \), is greater than the number of levels, \( N_S^R \geq N_\lambda \), and depends on the values of the resonance parameters \( \{ E_\lambda, \gamma_\lambda, B_c, E_{T}, a_c \} \) — though in a way that is invariant under change of boundary-condition \( B_c \),

- each neutral particle, odd angular momentum \( \ell_c \equiv 1 \pmod{2} \), channel adds at least one real analytic Brune pole below threshold,

- the number \( N_S^R \) of real analytic Brune poles is greater than the number \( N_\lambda \) of levels: \( N_S^R \geq N_\lambda \).

FIG. 4. Elemental Brune eigenproblem (51): comparison of solutions from definitions (39) versus (42), for angular momentum \( \ell_c = 1 \), neutral particles, using \( B_c = -\ell_c \), conversion zero threshold \( E_{T_0} \). Since both have a real sub-threshold poles, both will yield two solutions (crossing the \( E=E \) diagonal), one above and one below the discontinuity. If at threshold energy \( E_{T_0} \), the left hand side of (51) is above the \( E=E \) diagonal, then the above-threshold solutions from both definitions coincide. In any case, the sub-threshold solutions differ. Behavior is analogous for all odd angular momenta \( \ell_c \equiv 1(\text{mod} 2) \).
Proof. The proof follows the one of theorem 1. However, when considering the left-hand side of (33), the shift function is now defined from analytic continuation definition (42), which in general entails \( S_c(E) \) is a complex number. This entails the left-hand side of (33) is now a complex symmetric matrix. In general, a complex symmetric matrix is not diagonalizable, has no special properties on its spectrum, and we refer to reference literature on its Jordan canonical form and other properties [46–52]. Nonetheless, we know the left-hand side of (33) will be real-symmetric, thus diagonalizable, for real energies above threshold, which hints (but does not prove) it is probably a good assumption to assume the complex symmetric matrix to be non-defective in general. Regardless of the eigenvectors, we can search for the Brune poles \( \{ E_i \} \) by solving problem (37) directly (c.f. discussion around equation (51) in [23]). Here, the analytic properties of definition (42), established in lemma 3, entail the determinant in (37) is a meromorphic operator of \( \rho^2 \), which unfolds mapping (6) so that all the solutions of (37) live on one single sheet.

In the case of \( N_c \) massive neutral channels, the shift factor \( S_c(\rho) \) is a rational fraction in \( \rho^2 \) with a degree of \( \ell_c \) (in \( E \) space) in the denominator, where \( \ell_c \) is the angular momentum of the channel (c.f. table II and lemma 3 with table III). The search for the poles of the \( R_S \) operator (37) will then yield \( N_S \) complex Brune poles \( \{ E_i \} \in \mathbb{C} \) with \( N_S = N_\lambda + \sum_{c=1}^{N_c} \ell_c \), as stated in (46). The intuition behind this number \( N_S \) is that both the R-matrix (17) and the diagonal matrix of shift functions, \( S(E) := \text{diag} (S_c(E)) \), will each contribute their respective poles, \( N_\lambda \) and \( \sum_{c=1}^{N_c} \ell_c \) respectively, adding up to yield \( N_S = N_\lambda + \sum_{c=1}^{N_c} \ell_c \) solutions (46) to the determinant problem (37). We achieved a formal proof of result (46), though it is somewhat technical. It rests on the diagonal divisibility and capped multiplicities lemma 4, which we apply to the developed rational fraction det \( (R_S^{-1}(E)) \) in (37), or directly to (33), depending on whether \( N_\lambda \geq N_c \) or \( N_c \geq N_\lambda \). In the (most common) case of \( N_\lambda \geq N_c \), we develop det \( (R_S^{-1}(E)) = \text{det} (R^{-1} - S^0) \) by n-linearity: det \( (R^{-1} - S^0) = \text{det} (R^{-1}) \text{det} (I - R^{-1} S^0) \text{det} (I - R S^0) \), with \( \text{det} (I - R S^0) = 1 - \text{Tr} (R S^0) + \ldots + \text{Tr} (\text{Adj} (-R S^0)) - \text{det} (-R S^0) \), so that: det \( (R^{-1}) = \text{det} (R^{-1}) - \text{Tr} (\text{Adj} (R^{-1} S^0)) + \ldots - \text{Tr} (R^{-1} \text{Adj} (S^0)) + (-1)^{N_c} \text{det} (S^0) \). In the latter expression, \( R^{-1}(E) = \gamma^T (e - E I) \gamma^T \) has no poles, so its determinant is a polynomial det \( (R^{-1}(E)) \in \mathbb{C}[X] \). The rational fraction with greatest degree in the denominator is \( \text{det} (S^0(\gamma)) \in \mathbb{C}(X) \). For neutral particles \( S^0(\gamma) = S_c^0(E)^{\gamma} \), where the denominator is of degree \( \ell_c = \text{deg}(d_c(E)) \) in \( E \) space (c.f. table II), so that to rationalize the rational fraction det \( (R_S^{-1}(E)) \in \mathbb{C}[X] \), we must multiply it by the denominator of det \( (S^0(\gamma)) \), which is \( \prod_{c=1}^{N_c} d_c(E) \), a polynomial of degree \( \sum_c \ell_c \). That is \( \left( \prod_{c=1}^{N_c} d_c(E) \right) \times \text{det} (R_S^{-1}(E)) = \left( \prod_{c=1}^{N_c} d_c(E) \right) \times \text{det} (R^{-1}(E)) + \ldots + (-1)^{N_c} \prod_{c=1}^{N_c} s_c^0(E) \in \mathbb{C}[X] \). The dominant degree polynomial in this expression is \( \left( \prod_{c=1}^{N_c} d_c(E) \right) \times \text{det} (R^{-1}(E)) \). In this expression, the total degree of the polynomial is the sum of the degrees of the product terms. We readily have deg \( \left( \prod_{c=1}^{N_c} d_c(E) \right) = \sum_c \ell_c \). For the degree of the determinant term \( \text{det} (R^{-1}(E)) \), the application of diagonal divisibility and capped multiplicities lemma 4 stipulates that if \( E_{\lambda_1} = E_{\lambda_2} = \ldots = E_{\lambda_{N_\lambda}} \), this multiplicity \( m_\lambda \) of the resonance energy value \( E_\lambda \) will be capped by \( N_c \). In practice, this does not happen because the Wigner-Eisenbud resonance parameters \( E_\lambda \) are defined as different from each other \( E_\lambda \neq E_{\mu \neq \lambda} \). This is no longer true in the case \( N_c \geq N_\lambda \), where developing the determinant of (33) directly will similarly yield by n-linearity, and denoting  \( \Delta := e - E \mathbb{I} \) for clarity of scripture: \( \text{det} (\Delta - \gamma S^0(\gamma)) = \text{det} (\Delta) + \text{Tr} (\text{Adj} (\Delta) \gamma S^0(\gamma)) + \ldots - \text{Tr} (\Delta \text{Adj} (\gamma S^0(\gamma)) + (-1)^{N_\lambda} \text{det} (\gamma S^0(\gamma)) \). Again, in the latter expression the rational fractional with the highest-degree denominator is \( \text{det} (\gamma S^0(\gamma)) \in \mathbb{C}(X) \). Applying the diagonal divisibility and capped multiplicities lemma 4 to it commands that if there are various channels with the same \( S_c(E) \), for instance with the same \( \ell_c \) and \( \rho_{0c} \), their multiplicity of occurrence is capped by \( N_\lambda \) when rationalizing the fraction det \( (\gamma S^0(\gamma)) \in \mathbb{C}(X) \), so that \( Q(E) \times \text{det} (\gamma S^0(\gamma)) (E) \in \mathbb{C}[X] \) is a polynomial, with \( Q(E) := \left( \prod_{c=1}^{N_c} d_c(E) \right) \times \left( \prod_{c=1}^{N_c} \sum_{c \neq c'} d_c(E) \right) \). In the developed expression of the polynomial \( Q(E) \times \text{det} (\Delta - \gamma S^0(\gamma)) \), the dominant degree term is now: \( Q(E) \times \text{det} (\Delta) \), the degree of which is the sum of the degree of each term. The degree of \( \text{det}(\Delta) \) is \( N_\lambda \), whereas the degree of \( Q(E) \) is \( \text{deg}(Q(E)) = \sum_{c=1}^{N_c} \ell_c + \sum_{c=1}^{N_\lambda} \ell_c \). Hence, we find back the expression (46) to be proved: \( N_S = N_\lambda + \sum_{c=1}^{N_c} \ell_c \), but with the additional subtlety that the multiplicities (repeating occurrences) are capped, both for \( \sum E_\lambda \text{ multiplicity} \text{deg}(E_\lambda - \rho^2(E)) \) and for capped at \( N_\lambda \)

\[
\sum S_c \text{ multiplicity} \text{deg}(d_c(\rho(E)))
\]

so that the final, encompassed at \( N_\lambda \) count number of complex eigenvalues to Brune’s generalized eigenproblem (33) in the neutral channels case is:

\[
N_S = N_\lambda + \sum S_c \text{ multiplicity} \text{capped at } N_\lambda
\]
This behavior is depicted in figure 4.

A final technical note to state that this number $N_S$ of poles (47) is true in $E$ space, as we have showed in lemma 3 that definition (42) unfolds the Riemann sheet of (6). If we were performing this in $\rho$ space, we would thus simply multiply the degrees by 2. This is not true if we were searching for the poles of the Kapur-Peierls operator $R_1$, as the mapping of $\rho(E)$ is not one-to-one anymore. From table I, we would be able to perform the same analysis that yielded (47), but it would have to be in $\rho$ space, as we did to establish (76).

In the charged particles case, $S_c(E)$ has an infinity of poles (c.f. our discussion in section IV B). Extending our proof of (47) from the neutral particles to the charged particles ones would thus yield a countable infinity of complex Brune poles.

The key question is: how many of the $N_S$ complex Brune poles are real? To address it, we come back to theorem 1, the number of real analytic Brune poles, will depend on the R-matrix parameters $\{\lambda, \gamma, a_\lambda\}$, including (25) into (37)). We illustrate various such cases in figure 5. However, each neutral particle channel with odd angular momenta (c.f. section III B 2) introduces a shadow Brune pole is on the same, unique sheet. The same behavior will be observed for all odd angular momenta $\ell_c \equiv 1 \bmod 2$. (50)

We here have a sum of products of $m$ terms; thus, the $R_j(z)$ never appear more than $m$ times in each product – nor more than their multiplicity in $\det(D)(z)$. It thus suffices to account for each $P_j(z)$ a number of times that is the maximum between its multiplicity and $m$ in order to rationalize the $\det(MDM^T) \in \mathbb{C}(X)$ fraction. 

Importantly, since both shift function $S_c(E)$ definitions (39) and (41) coincide above threshold, the solutions to (33) will be the same above thresholds. The discrepancy in the values of the Brune parameters, solutions to (33), will only differ when certain channels have to be considered below threshold: $S_c(E)$ with $E < E_{T_r}$. To illustrate these differences, let us consider the simple example of a one-level, one-channel neutral particle interaction, with a zero-threshold $E_{T_r} = 0$, and set about solving the Brune generalized eigenproblem (33), which here takes the simple scalar form:

$$E_\lambda - \gamma_{\lambda,c} S_c(E) - B_\lambda \gamma_{\lambda,c} = 0$$

In figures 4 and 5, we plotted the left and right hand side of this elemental Brune eigenproblem (51), for both definitions (39) and (42) of the shift function $S_c(E)$, for various values of resonance parameters $\{E_\lambda, \gamma_{\lambda,c}\}$ and the convention $B_\lambda = -\ell_c$, for different angular momenta $\ell_c$.

In the case of $\ell_c = 1$, depicted in figure 4, one can observe that the real sub-threshold pole engendered by odd angular momenta (c.f. section III B 2) introduces a sub-threshold Brune parameter, where the left-hand side of (51) crosses the $E = E$ identity line. In the case of the Lane & Thomas legacy definition (39), this sub-threshold shadow Brune pole is on the $\{E, -\}$ sheet of mapping (2), whereas for analytic continuation definition (42) it is on the same, unique sheet. The same behavior will be observable for all odd angular momenta $\ell_c \equiv 1 \bmod 2$.

In the case of $\ell_c = 2$, depicted in figure 5, the non-purely-imaginary poles $\{\omega_a, \omega_a^*\} \not\in \mathbb{R}$ (c.f. lemma 3 and table III) will impact the shift function $S_c(\rho_c)$ in ways that may
FIG. 5. Elemental Brune eigenproblem (51): comparison of solutions from definitions (39) versus (42), for angular momentum \( \ell_c = 1 \) case, where the analytic shift function takes the wavenumber dependence, \( S(\rho) = \frac{1}{1 + \rho^2} \), and thus the poles of the \( R_S \) operator are nothing but the solutions to \( \frac{E - \tilde{E}}{\gamma_{\lambda,c}} + B + \frac{1}{1 + \rho^2} (E - E_{T_c}) = 0 \). The fundamental theorem of algebra then guarantees this problem has \( N_S = 2 \) complex solutions, not \( N_\lambda = 1 \). The surprising part is that both are real poles: one above and one below threshold, which again stems from the fact the number of roots \( \{\omega_c\} \) is odd and that their symmetries thus require one pole to be exactly imaginary (in wavenumber space), as explained in section III B 2. For \( \ell_c = 2 \), we would have \( S_2(E) = \frac{3E + 2\omega^2}{\omega^2 + 3E + E^2} \), so that the fundamental theorem of algebra commands (51) will have \( N_S = 3 \) solutions, verifying the \( N_S = N_\lambda + \sum_{c=1}^{N_\lambda} \ell_c \) complex poles we establish in (46). In the general charged-particles case, the shift factor \( S_c(\rho) \) is no longer a rational fraction in \( \rho^2 \) but is a meromorphic operator in \( \rho^2 \) with an infinity of poles (c.f. lemma 3). This means that, in general, there exist \( N_\lambda \leq N_S \leq \infty \) complex poles of the \( R_S \) operator, and that at least \( N_\lambda \) of them are real.

When the left-hand side of (51) crosses the \( E = E \) identity line above threshold, the branch Brune poles coincide with the analytic Brune poles, as can be observed in figures 4 and 5. Since the shift function \( S_c(E) \) is continuous and monotonically increasing above threshold, the question is whether the eigenvalues of the left-hand side of (33) are above the \( E = E \) line at the threshold value: \( E = E_{T_c} \). If yes, then it would mean that past the last threshold there will be exactly \( N_\lambda \) solutions to (33). However, nothing guarantees \textit{a priori} that all the eigenvalues of the left hand side of (33) are above the \( E = E \) at the last threshold. From solving the elemental Brune problem (51), we observed that it seems to require negative resonance levels \( E_\lambda < 0 \) to induce the left-hand side of (33) to be below the \( E = E \) line at the threshold value, as illustrated in figures 4 and 5. When this happens, the Brune poles will be sub-threshold, and thus depend on the (39) or (42) definition for the shift function \( S_c(E) \). However, the fact that different channels will have different threshold levels \( E_{T_c} \neq E_{T_c'} \), and that nothing stops R-matrix parameters from displaying negative resonance levels \( E_\lambda < 0 \), mean no definitive conclusion can be reached as to the number of real Brune parameters.

or may not produce additional real solutions \( \{ \tilde{E}_i \} \in \mathbb{R} \) to the generalized eigenproblem (33). This behavior is reported in figure 5, where one can observe that, depending on the R-matrix parameter values \( \{ E_\lambda, \gamma_{\lambda,c}, B_c \} \), there are either one, two (tangential for the analytic continuation definition), or three solutions to the Brune generalized eigenproblem (51). For instance, one can see that definition (39) can yield situations with two sub-threshold branch Brune poles – one on the \( \{ E, + \} \) branch and one shadow pole (i.e. on the \( \{ E, - \} \) branch) – or with two sub-threshold shadow Brune poles – both sub-threshold on the \( \{ E, - \} \) branch – or situations where only one, above-threshold solution is produced. On the other hand, analytic continuation definition (42) can also yield one, two (tangentially) or three solutions, depending on the sub-threshold behavior and the resonant parameters eigenvalues \( \{ E_\lambda, \gamma_{\lambda,c}, B_c \} \). The number of real solutions \( \{ \tilde{E}_i \} \in \mathbb{R} \) to the Brune generalized eigenproblem (33) will thus depend on the R-matrix parameters, and is in general comprised between \( N_\lambda \) and \( N_S \).
4. Choice of Brune poles

Brune defined his alternative Brune parameters in (34) and (35) by building the square matrix \( g \), and then inverting it to guarantee (36) (c.f. section III.B.1). We just demonstrated in theorems 1 and 2 that there are in general more Brune poles \( N_S \) – either branch Brune poles or analytic Brune poles – than the number \( N_\lambda \) of resonance levels: \( N_S \geq N_\lambda \). Yet the fact that there are more than \( N_\lambda \) solutions to (33) implies the \( g := [g_1, \ldots, g_i, \ldots, g_{N_S}] \) matrix, composed of the \( N_S \) solutions to Brune’s eigenproblem (33), is in general not square, and could even be infinite if \( N_S = \infty \) (Coulomb channels). This brings two critical questions: 1) do these additional Brune poles impede us from well defining the Brune parameters? 2) can we still uniquely define the Brune poles?

We here demonstrate in theorem 3 the striking property that choosing any finite set of at least \( N_\lambda \) different solutions from the \( N_\lambda \leq N_S \leq \infty \) solutions of Brune’s eigenproblem (33), suffices, under our new extended definition (52), to properly describe the \( R \)-matrix scattering model.

**Theorem 3. Choice of Brune poles**

If we generalize Brune’s definition (35) of the physical level matrix to its pseudo-inverse \( \tilde{A}^+ \), setting:

\[
\tilde{A}^+ := g^T A^{-1} g 
\]  

then the choice of any number \( N_S \) of Brune poles, solutions to the Brune generalized eigenproblem (33), will reconstruct the scattering matrix \( U(E) \), as long as we choose at least \( N_\lambda \) solutions: \( N_S \geq N_\lambda \).

**Proof.** The proof rests on the pseudo-inverse property for independent columns and rows, and applies it to the \( g := [g_1, \ldots, g_i, \ldots, g_{N_S}] \) matrix, constructed by choosing \( N_S \) solutions of the generalized eigenproblem (33). If \( N_S \geq N_\lambda \), then \( g \) has independent rows so that its pseudo-inverse will yield: \( \tilde{A} = g^+ A g^{+T} \). This property in turn entails (36) is satisfied, and thus (32) stands, leaving unchanged the Kapur-Peierls operator \( R_L \), and hence fully representing the scattering matrix \( U(E) \). \( \square \)

Critically, \( N_\lambda \) real solutions to (33) can always be found – as shown in theorems 1 and 2 – meaning the Brune parametrization is always capable of fully reconstructing the scattering matrix energy behavior with real parameters through generalized pseudo-inverse definition (52). It is well defined.

Yet, if any choice of \( N_\lambda \) Brune poles will yield the same scattering matrix \( U(E) \) through definition (52), this choice is *a priori* not unique. Can we define some conventions on the choice of Brune parameters to make them unique? Under the legacy Lane & Thomas definition (39), this can readily be achieved by neglecting the shadow poles and restraining the search to the principal sheet \( \{ E_i, \ldots, + \} \), for all \( N_c \) channels, where we have shown in theorem 1 that one will find exactly \( N_\lambda \) poles. Under the analytic continuation definition (42), one can still uniquely define the \( N_\lambda \) “first” solutions in the following algorithmic way: one starts the search by diagonalizing, at the last threshold energy (greatest \( E_T \) value), the left-hand side of (33). If all the eigenvalues are above the \( E = E_T \) line, then increase the energy until the eigenvalues cross the \( E = E_T \) diagonal, and we will have \( N_\lambda \) uniquely defined real analytic Brune poles. If at the first threshold some eigenvalues are below the \( E = E_T \) line (as we saw could happen if some resonance energies are negative \( E_\lambda < 0 \)), then we can decrease the energy values until those cross the \( E = E_T \) line for the first time, and stop the search there, thus again uniquely defining \( N_\lambda \) analytic Brune poles. This foray into the algorithmic procedure for solving (42) gives us the occasion to point to the vast literature on methods to solve non-linear eigenvalue problems, in particular [53].

In the end, though we argue that the physically correct definition for the shift function \( S_i(E) \) ought to be through analytic continuation (42), both approaches enable to set conventions that will uniquely determine \( N_\lambda \) real Brune poles.

C. Complex invariant \( R_L \) parameters: Siegert-Humblet expansion in radioactive states

The previous section describes how Brune transformed the real Wigner-Eisenbud resonance parameters \( \{ E_\lambda, \gamma_{\lambda,c}, B_c \} \) into a set of real boundary-condition-independent parameters \( \{ \tilde{E}_i, \tilde{\gamma}_{i,c} \} \). As we saw, this comes at the cost of having to set a convention to uniquely choose \( N_\lambda \) Brune parameters (c.f. theorem 3), but at the gain of producing a set of real parameters \( \{ a_c, \tilde{E}_i, \tilde{\gamma}_{i,c}, E_T \} \) that entirely characterizes the scattering matrix \( U \) and thus the reaction.

In this section we provide new insights into another way of parametrizing the \( R \)-matrix model that leads to complex invariant parameters through \( R_L \): the Siegert-Humblet expansion into radioactive states (c.f. sections IX.2.c-d-e p.297-298 in [5]). As we will see, these parameters have the advantage of being unique and invariant to boundary condition \( B_c \), as well as easily transformed under a change of channel radius \( a_c \) (theorem 4 section IV), and of locally untangling the energy dependence of the scattering matrix as a simple sum of poles and residues. This comes at the cost of greater parameter complexity: the parameters are complex and strongly intertwined; they live on a sub-manifold of the multi-sheeted Riemann surface that the wavenumber-energy mapping (6) introduces; and they only allow for a local characterization of the scattering matrix \( U \), not a global one \( \forall E \in \mathbb{C} \).
1. Definition of Siegert & Humblet $R_L$ parametrization

At the heart of the Siegert-Humblet parametrization stands the Kapur-Peierls operator, $R_L$, defined in (20):

$$R_L^{-1} := R^{-1} - L^0 = R^{-1} + B - L = \gamma^T A \gamma$$

This definition is analogous to Brune’s $R_S$ in (38). By analytically continuing the $R$ (17) and $L$ (10) operators to complex energies $E \in \mathbb{C}$, the Kapur-Peierls matrix $R_L$ becomes a locally meromorphic operator. The poles of this meromorphic operator can be assumed to have a Laurent expansion of order one, as we will discuss in section V.C.1. Since the Kapur-Peierls $R_L$ operator is complex-symmetric, this entails its residues at any given pole value $E_j \in \mathbb{C}$ are also complex symmetric. For non-degenerate eigenvalues $E_j \in \mathbb{C}$, the corresponding residues are rank-one and expressed as $r_j r_j^T$, while for degenerate eigenvalues $E_j \in \mathbb{C}$ of multiplicity $M_j$, the corresponding residues are rank-$M_j$ and expressed as $\sum_{m=1}^{M_j} r_j^m r_j^{m^T}$. On a given domain, the Mittag-Leffler theorem [54, 55] then states that $R_L$ locally takes the form, in the vicinity $V(E)$ of any complex energy $E \in \mathbb{C}$ away from the branch points (threshold energies $E_{T_k}$) of mapping (6), of a sum of poles and residues and a holomorphic entire part $\text{Hol}_R(L)(E)$:

$$R_L(E) = \sum_{j=1}^{M_j} \frac{\sum_{m=1}^{M_j} r_j^m r_j^{m^T}}{E - E_j} + \text{Hol}_R(L)(E)$$

or, in the particular (but usual) case where $E_j$ is a non-degenerate eigenvalue (with multiplicity $M_j = 1$),

$$R_L(E) = \sum_{j=1}^{M_j} \frac{r_j r_j^T}{E - E_j} + \text{Hol}_R(L)(E)$$

This is the Siegert-Humblet expansion into so-called radioactive states [24, 56–58] — equivalent to equation (2.16) of section IX.2.c. in [5] where we have modified the notation for greater consistency ($E_j$ corresponds to $H_0$ of [5] and $r_j$ corresponds to $\omega_j$) since there are more complex poles $E_j$ than real energy levels $E_N$. The Siegert-Humblet parameters are then the poles $\{E_j\}$ and residue widths $\{r_j\}$ of this complex resonance expansion of the Kapur-Peierls operator $R_L$.

The Gohberg-Sigal theory provides a method for calculating these poles and residues by solving the generalized eigenvalue problem [59]:

$$R_L^{-1}(E) |_{E=E_j} q_j = 0$$

i.e. solving for the poles $\{E_j\}$ of the Kapur-Peierls matrix $R_L$ operator and their associated eigenvectors ($q_j$). The poles are complex and usually decomposed as:

$$E_j := E_j - i \frac{\Gamma_j}{2}$$

It can be shown (c.f. discussion section IX.2.d pp.297–298 in [5], or section 9.2 eq. (9.11) in [2]) that fundamental physical properties (conservation of probability, causality and time reversal) ensure that the poles reside either on the positive semi-axis of purely-imaginary $k_c \in \mathbb{IR}^+$ — corresponding to bound states for real sub-threshold energies, i.e. $E_j < E_{T_k}$, 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 $M_j = \dim(\text{Ker} (R_L^{-1}(E_j)))$ be the dimension of the nullspace of the Kapur-Peierls operator at pole value $E_j$ — that is $M_j$ is the geometric multiplicity. We can thus write $\text{Ker} (R_L^{-1}(E_j)) = \text{vect} (q_j^1, ..., q_j^{M_j})$.

As we discuss in section V.C.1, it is physically reasonable to assume that the geometric and algebraic multiplicities are equal (semi-simplicity condition), which entails a Laurent development of order one for the poles — i.e. no higher powers of $\frac{1}{E - E_j}$ in expansion (53). Since $R_L$ is complex symmetric, if we assume we can find non-quasi-null eigenvectors solutions to (55) — that is $\forall (j,m), \ q_j^m q_j^{m^T} \neq 0$ so it is non-defective [46–52] — then the Gohberg-Sigal theory can be adapted to the case of complex symmetric matrices to normalize the rank-$M_j$ residues of $R_L$ matrix as:

$$\sum_{m=1}^{M_j} r_j^m r_j^{m^T} = \sum_{m=1}^{M_j} q_j^m q_j^{m^T} \left( \frac{\partial R_L^{-1}}{\partial E} |_{E=E_j} \right) q_j^m$$

In practice, we are most often presented with non-degenerate states where $M_j = 1$, meaning the kernel is an eigenline $\text{Ker} (R_L^{-1}(E_j)) = \text{vect} (q_j)$, which entails rank-one residues normalized as:

$$r_j r_j^T = \frac{q_j q_j^T}{q_j^T \left( \frac{\partial R_L^{-1}}{\partial E} |_{E=E_j} \right) q_j}$$

The residue widths $\{r_j^m\}$, here called radioactive widths, can thus directly be expressed as:

$$r_j^m = \frac{q_j^m}{\sqrt{q_j^m q_j^{m^T} \left( \frac{\partial R_L^{-1}}{\partial E} |_{E=E_j} \right) q_j^m}}$$

where $\left( \frac{\partial R_L^{-1}}{\partial E} |_{E=E_j} \right)$ can readily be calculated by means of property (27) to yield

$$\left. \frac{\partial R_L^{-1}}{\partial E} \right|_{E=E_j} = \frac{\partial R^{-1}}{\partial E}(E_j) - \frac{\partial L}{\partial E}(E_j)$$

with

$$\frac{\partial R^{-1}}{\partial E} = -R^{-1} \gamma^T (e - EI)^{-2} \gamma R^{-1}$$
The radioactive poles, \( \{ \mathcal{E}_j \} \), and residue widths, 
\[
\left\{ r_j^m = \left[ r_{j,c_1}^m, \ldots, r_{j,c_l}^m, \ldots, r_{j,c_{\lambda_c}}^m \right]^T \right\},
\]
are the Siegert-Humblet parameters. They are complex and locally untangle the energy dependence into the sum of poles and residues (53). Additional discussion on these poles and residues can be found in [5], sections IX.2.c-e p.297-298, or in [24, 56–58]. Focusing on invariance, since the Kapur-Peierls matrix \( R_L \) is invariant to a change in boundary conditions \( B_c \) — c.f. equations (24) and (25) — this entails the radioactive poles \( \{ \mathcal{E}_j \} \) and widths \( \{ r_j \} \) are boundary condition \( B_c \) independent. We will also prove (c.f. theorem 7) that the poles \( \{ \mathcal{E}_j \} \) are exactly the poles of the scattering matrix \( U(E) \), which also makes them invariant to channel radii \( \{ a_c \} \). From (19), the radioactive widths \( \{ r_j \} \) are not themselves invariant in change of channel radius \( a_c \), but we will also show in theorem 4 section IV how to transform them under a change of channel radius \( a_c \).

2. Level matrix \( \mathbf{A}(E) \) approach to Siegert & 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 \( \{ a_c, B_c, \gamma_{\lambda_c}, E_{\mathcal{L}_c}, E_{T_c} \} \) is through the level matrix \( \mathbf{A} \). This strongly mirrors Brune’s generalized eigenvalue problem (33) in that we search for the poles and eigenvectors of the level matrix operator \( \mathbf{A} \):

\[
\mathbf{A}^{-1}(E)|_{E = \mathcal{E}_j} \mathbf{b}_j = 0
\]

i.e. solve for the eigenvalues \( \{ \mathcal{E}_j \} \) and associated eigenvectors \( \{ \mathbf{b}_j \} \) that satisfy:

\[
[\mathbf{e} - \gamma (\mathbf{L}(\mathcal{E}_j) - \mathbf{B}) \gamma^\top] \mathbf{b}_j = \mathcal{E}_j \mathbf{b}_j
\]

This problem is analogous to (33), replacing the shift factor \( \mathbf{S} \) with the outgoing-wave reduced logarithmic derivative \( \mathbf{L} \).

Again, the same hypotheses as for \( R_L \) in section III C 1 allow us to adapt the Gohberg-Sigal theory to the case of complex symmetric operators to locally yield the following formula for the normalized residues in the Mittag-Leffler expansion of the level matrix:

\[
\mathbf{A}(E) = \sum_{j \geq 1}^M \frac{\mathbf{a}_j^m \mathbf{a}_j^{m\top}}{E - \mathcal{E}_j} + \text{Hol}_\mathbf{A}(E)
\]

In the most frequent case of non-degenerate eigenvalues to (62), this yields rank-one residues as:

\[
\mathbf{A}(E) = \sum_{j \geq 1}^M \frac{\mathbf{a}_j \mathbf{a}_j^{\top}}{E - \mathcal{E}_j} + \text{Hol}_\mathbf{A}(E)
\]

Again, under non-quasi-null eigenvectors assumption \( \mathbf{b}_j^m \mathbf{b}_j^m \neq 0 \), Gohberg-Sigal theory ensures the residues are normalized as:

\[
a_j^m a_j^{m\top} = \frac{\mathbf{b}_j^m b_j^{m\top}}{\left( \frac{\partial \mathbf{A}^{-1}}{\partial E} \right)_{E = \mathcal{E}_j} b_j^m}
\]

which is readily calculable from

\[
\frac{\partial \mathbf{A}^{-1}}{\partial E}(\mathcal{E}_j) = -\mathbf{I} - \gamma \frac{\partial \mathbf{L}}{\partial E}(\mathcal{E}_j) \gamma^\top
\]

Plugging (64) into (20), and invoking the unicity of the complex residues, implies the radioactive widths (59) can be obtained as

\[
r_j^m = \gamma^\top a_j^m
\]

This is an interesting and novel way to define the Siegert-Humblet parameters, which is similar to the parameter definition of Brune (34). From this perspective, the Brune parameters appear as a special case that leave the Siegert-Humblet level-matrix parameters boundary condition \( B_c \) invariant. Indeed, the defining property of Brune’s parameters (32) means we can search for the Siegert-Humblet expansion of the Brune parameters, simply by proceeding as in (62) with Brune’s alternative physical level matrix \( \tilde{\mathbf{A}} \) from (29) or (52):

\[
\tilde{\mathbf{A}}^{-1}(E)|_{E = \mathcal{E}_j} \tilde{\mathbf{b}}_j = 0
\]

The exact same Gohberg-Sigal procedure can then be applied to the Mittag-Leffler expansion of Brune’s \( \tilde{\mathbf{A}} \) physical level matrix, in the vicinity \( \mathcal{V}(E) \) of \( E \in \mathbb{C} \) away from branch points \( \{ E_{T_c} \} \),

\[
\tilde{\mathbf{A}}(E) = \sum_{j \geq 1}^M \frac{\sum_{m=1}^M \tilde{a}_j^m \tilde{a}_j^{m\top}}{E - \mathcal{E}_j} + \text{Hol}_\tilde{\mathbf{A}}(E)
\]

yielding the normalized residue widths:

\[
\tilde{a}_j^m \tilde{a}_j^{m\top} = \frac{\tilde{b}_j^m b_j^{m\top}}{\left( \frac{\partial \tilde{\mathbf{A}}^{-1}}{\partial E} \right)_{E = \mathcal{E}_j} b_j^m}
\]

where (29) can be used to calculate the energy derivative. Then, when plugging (71) into (32), we obtain the relation between the Brune and the Siegert-Humblet \( R \)-matrix parameters:

\[
r_j^m = \gamma^\top \tilde{a}_j^m
\]

This relation (72) is especially enlightening when compared to (68) from the viewpoint of invariance to boundary condition \( B_c \). Indeed, we explained that the Siegert-Humblet parameters \( \{ \mathcal{E}_j, r_j^m \} \) are invariant with a change of boundary condition \( B_c \rightarrow B'_c \). This is however not true of the level matrix residue widths \( \{ a_j^m \} \)
from (66). Thus, we can formally write this invariance by differentiating (68) with respect to $B_c$ and noting that 
$$ \frac{\partial a_m^j}{\partial B} = 0 $$ 
yielding:

$$ 0 = \frac{\partial \gamma^T}{\partial B} a_m^j + \gamma^T \frac{\partial a_m^j}{\partial B} $$

(73)

This new relation links the variation of the Wigner-Eisenbud widths $\gamma_{\lambda,c}$ at level values $E_j$, to the variation of the level matrix residue widths $a_m^j$, at pole values $E_j$ under change of boundary condition $B_{c^{'}}$. Since transformations (23) detail how to perform $\frac{\partial \gamma^T}{\partial B}$, equation (73) could be used to update $a_m^j$ under a change $B_c \rightarrow B_{c^{'}}$.

Another telling insight from relation (73) is when we apply it to the relation between the Brune parameters and the Siegert-Humblet residue widths (72). Then, since the Brune parameters $\gamma$ are invariant to $B_c$, the same differentiation as in (73) now yields zero derivatives,

$$ 0 = \hat{\gamma}^T \frac{\partial a_m^j}{\partial B} $$

(74)

Though this is obvious from the fact that Brune’s physical level matrix $\tilde{A}$ is invariant under change of boundary condition, it does present the Brune parametrization as the one which leaves the level residue widths $\{a_m^j\}$ invariant to $B_c$ when transforming to Siegert-Humblet parameters though (72).

Conversely, the Siegert-Humblet Kapur-Peierls matrix resonance expansion (54) completes Brune’s parametrization in that it generates the boundary condition $B_c$ independent poles $\{E_j\}$ and radioactive widths $\{r_j\}$ that explicitly invert Brune’s alternative physical level matrix (29) to yield (70).

In practice we are most often presented with the non-degenerate case of rank-one residues (eigenvalue multiplicity of $M_j = 1$), 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.

3. $R_l$: complex parameters: local expansion, multi-sheeted Riemann surface, poles & residues

We here discuss some subtle points in line with section III B 2, concerning the continuation of $R$-matrix operators to complex energies $E \in \mathbb{C}$, which is required in the procedure to calculate the Siegert-Humblet parameters.

We first start with a numerical note. Numerically, solving the generalized eigenvalue problems (55) or (63) falls into the well-known class of nonlinear eigenvalue problems, for which algorithms we direct the reader to Heinrich Voss’s chapter 115 in the Handbook of Linear Algebra [53]. We will just state that instead of the Rayleigh-quotient type of methods expressed in [53], it can sometimes be computationally advantageous to first find the poles $\{E_{j}\}$ by solving the channel determinant problem, det $\left( R^{-1}_l(E) \right)_{E = E_{j}} = 0$, analogous to (37), or the corresponding level determinant one, det $\left( A^{-1}(E) \right)_{E = E_{j}} = 0$, and then solve the associated linear eigenvalue problem. Methods tailored to find all the roots of this problem where introduced in [60], or in equations (200) and (204) of [61]. Notwithstanding, from a numerical standpoint, having the two approaches is beneficial in that solving (55) will be advantageous over solving (63) when the number of levels $N_{\lambda}$ far exceeds the number of channels $N_c$, and conversely.

Let us now provide some remarks on the thorny question of the multi-sheeted nature of the problem. When solving problem (55), or (63), to obtain the Siegert-Humblet poles $\{E_{j}\}$ and residues $\{r_{j}\}$, or $\{a_{j}\}$, it is necessary to compute the $L^0$ matrix function $L^0(E) := \hat{L}^0(\rho(E))$ for complex energies $E \in \mathbb{C}$. As discussed in II A, mapping (6) generates a multi-sheeted Riemann surface with $2^{N_{\lambda}}$ branches (with the threshold values $E_{T_{\lambda}}$ as branch points), corresponding to the choice for each channel $c$, of the sign of the square root in $\rho(E)$. This means that when searching for the poles, one has to keep track of these choices and specify for each pole $E_j$ on what sheet it is found. Every pole $E_j$ must thus come with the full reporting of these $N_c$ signs, i.e.

$$ \{E_j, +, +, - , \ldots , +, - \} $$

(75)

The $\{E_j, +, +, \ldots , +, + \}$ sheet is called the physical sheet, and we here call the poles on that sheet the principal poles. All other sheets are called unphysical 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 [44], and G. Hale there introduced a quantity called strength of a pole (c.f. eq. (7) in [44], or paragraph after eq. (2.11) XI.2.b, p.306, and section XI.4, p.312 in [5]) to quantify the impact a pole $E_j$ will have on resonance behavior, by comparing the residue $r_{j,c}$ to the Wigner-Eisenbud widths $\gamma_{\lambda,c}$.

As discussed in section III B, there is an ambiguity of definitions for the shift and penetration functions, which in turn entail various possible Brune parameters. When solving (55) or (63) for the Siegert-Humblet poles and residues $\{E_j, r_{j,c}\}$, there are no such ambiguities on the definition of $L$. From (9), we extend $L(E)$ to complex energies by simply performing analytic continuation of the outgoing wave functions $O_{c}(\rho_{E})$, as for lemma 1 in section II B. This means the Siegert-Humblet parameters are uniquely defined, as long as we specify for each channel $c$ what sheet of the Riemann surface from mapping (6) was chosen, as in (75).

As it was the case for the Brune parameters, which counted more solutions than levels ($N_{S} \geq N_{\lambda}$), there are more Siegert-Humblet poles $\{E_{j}\}$ than Wigner-Eisenbud
levels \( \{E_\lambda \} \). For massive neutral particles, by proceeding in an analogous way as for (47), applying the diagonal divisibility and capped multiplicities lemma 4 to the determinant of the Kapur-Peierls operator \( R_L \) in (55) – but this time in \( \rho_c \) space (c.f. comment after (47) in proof of theorem 3) – and then looking at the order of the resulting rational fractions in \( \rho_c \) and the number of times one must square the polynomials to unfold all \( \rho_c = \pm \sqrt{\tau} \) sheets, we where able to establish that the number \( N_L \) of poles in wavenumber \( \rho \)-space is:

\[
N_L = \left( 2N_\lambda + \sum_{c=1}^{N_c} \ell_c \right) \times 2^{(N_{E_T} + N_{E_T}^*) - 1} \tag{76}
\]

where \( N_{E_T} \neq E_{T,j} \) designates the number of different thresholds (including the obvious \( E_T = 0 \) zero threshold). Again, as for (47), one should add the precision that in the sum over the channels in (76), the multiplicity of eventual \( L_c(\rho_c) \) repeated over many different channels \( \ell_c(\rho_c) = L_c(\rho_c) = \ell_c(\rho_c) \) is capped by \( N_\lambda \), 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 \( \mathcal{J}^\pi \)). One can observe that the number \( N_j \) of Siegert-Humblet poles adds-up the number of levels \( N_L \) and the number of poles of \( L \) which is \( \sum_{c=1}^{N_c} \ell_c \) for neutral massive particles, and is infinite in the Coulomb case, c.f. discussion in section IV). Moreover, \( N_j \) is duplicated with each new sheet of the Riemann surface from mapping (6) — that is associated to a new threshold, hence the \( N_{E_T} \neq E_{T,j} \). Interestingly, comparing \( N_j \) from (76) with the \( N_S \) Brune poles from (46) — which are in \( E \)-space and must thus be doubled to obtain the number of \( \rho \)-space poles — we note that the analytic continuation of the shift factor \( S \) adds a virtual pole per each pole of \( L \) when unfolding the sheets of (mapping 6) by being a function of \( \rho^2(\cal E) \). This can be readily observed in our trivial one level one p-wave (\( \ell = 1 \)) channel, where \( S(\cal E) = -\frac{1}{1 + \rho^2(\cal E)} \) introduces two poles at \( \rho(\cal E) = \pm i \), while \( L(\cal E) = \frac{-1 + \rho(\cal E) + \rho^2(\cal E)}{1 - \rho(\cal E)} \) only counts one pole, at \( \rho(\cal E) = i \).

It is important to grasp the meaning of the Mittag-Leffler expansion (54) — or (64) and (70). These are local expressions in that the branch-point structure of the Riemann sheet does not allow these Mittag-Leffler expansions to hold for all complex energy \( E \in \mathbb{C} \). However, away from the branch-points \( E_T \), the form locally stands, and the holomorphic part then has an analytic expansion \( \text{Hol}_{R_L}(\cal E) \): \( \sum_{n \geq 0} c_n E^n \), which means in a neighborhood \( V(\cal E) \) of \( E \in \mathbb{C} \) away from the thresholds \( \{E_T\} \) the following expansion holds:

\[
R_L(\cal E) = \sum_{j \geq 1} \frac{r_j \Gamma_j}{\cal E - \cal E_j} + \sum_{n \geq 0} c_n E^n \tag{77}
\]

This has two major consequences for the Siegert-Humblet expansion. First, contrarily to Brune’s parameters \( \{ \tilde{E}_j, \tilde{\gamma}_j,\} \), the Siegert-Humblet set of poles and radiocative widths \( \{ \xi_j, \nu_j \} \) do not suffice to uniquely determine the energy behavior of the scattering matrix \( U(\cal E) \): one needs to locally add the expansion coefficients \( c^n_{n,c} \) of the entire part \( \text{Hol}_{R_L}(\cal E) \): \( \sum_{n \geq 0} c_n E^n \). Second, since the set of coefficients \( \{ c_n \} \) is a priori infinite (and the poles set is too for 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 expanding the number of \( \{ \xi_j \} \) by \( \{ \nu_j \} \) at the order of the truncation \( N_{V(\cal E)} \) in \( \{ c_n \} \). In practice, this means that to compute the scattering matrix one needs to provide the Siegert-Humblet parameters \( \{ \xi_j, r_j, c \} \), cut the energy domain of interest into local windows \( V(\cal E) \) away from threshold branch-points \( \{ E_T \} \), and provide a set of local coefficients \( \{ c_n \} \) for each window.

4. Linking the R-matrix parametrization to the Humblet-Rosenfeld scattering matrix expansion

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 \( R_L \), through (55) and (59). Plugging its associated expansion (54) into the expression of the scattering matrix (19) then yields the Mittag-Leffler expansion of the scattering matrix:

\[
U(\cal E) = w \sum_{j \geq 1} \frac{u_j u_j^\dagger}{\cal E - \xi_j} + \text{Hol}(\cal E) \tag{78}
\]

where \( w := \text{wronskian} (7) \), and the scattering residue widths \( u_j \) are defined as:

\[
u_j := \left[ \rho^{1/2} O^{-1} \right]_{E=\xi_j} \cal E_j \tag{79}
\]

In writing (78), we have used the fact that all the resonances of the scattering matrix \( U(\cal E) \) come from the Kapur-Peierls poles \( \{ \xi_j \} \): the poles \( \{ \omega_k \} \) of the outgoing wave function \( O(\cal E) \) cancel out in (19) and are thus not present in the scattering matrix, this we demonstrate in theorem 6, section V C. Cauchy’s residues theorem then allows us to evaluate the residues at the pole value to obtain (79). As for (54), if a resonance were to be degenerate with multiplicity \( M_j \), the residues would no longer be rank-one, but instead the scattering matrix residue associated to pole \( \xi_j \) would be \( \sum_{m=1}^{M_j} u_j^m u_j^m \), with \( u_j^m := \left[ \rho^{1/2} O^{-1} \right]_{E=\xi_j} \cal E_j^m \).

Expression (78) exhibits the advantage that the energy dependence of the scattering matrix \( U(\cal E) \) is untangled in a simple sum. All the resonance behavior stems from the complex poles and residue widths \( \{ \xi_j, u_j, c \} \), 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 $\text{Hol}_U(E)$, which can be expanded in various forms, for instance analytically (80).

This establishes the important bridge between the R-matrix parametrizations and the Humblet-Rosenfeld expansions of the scattering matrix. More precisely, Mittag-Leffler expansion (78) is identical to the Humblet-Rosenfeld expansions (10.22a)-(10.22b) in [2] for the neutral particles case, and (5.4a)-(5.4b) in [16] 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 [15]. In particular, the poles $\{E_j\}$ from (56), found by solving (55), are exactly the ones defined by equations (9.5) and (9.8) in [2]. The scattering residue widths $\{u_{j,c}\}$, calculated from (79), then correspond to the Humblet-Rosenfeld complex residues (10.12) in [2], from which they build their quantities $\{G_{c,n}\}$ appearing in expansions (10.22a)-(10.22b) in [2], or (5.4a)-(5.4b) in [16]. Finally, the holomorphic part $\text{Hol}_U(E)$ corresponds to the regular function $Q_{c,c'}(E)$ defined between (10.14a) and (10.14b) in [2].

Just as Humblet and Rosenfeld did with $Q_{c,c'}(E)$ in section 10.2 of [2] and section 4 of [16], we do not give here an explicit way of calculating this holomorphic contribution $\text{Hol}_U(E)$ other than stating that it is possible to expand it in various ways. Far from a threshold, an analytic series in $E$ can stand:

$$\text{Hol}_U(E) = \sum_{n \geq 0} s_n E^n$$

In the immediate vicinity of a threshold, the asymptotic threshold behavior will prevail (for massive particles, $U_{c,c} \sim k_c^{\ell} + k_c^\prime$, c.f. eq. (10.5) in [2], or [62]), yielding an expansion of the form:

$$\text{Hol}_U(E) = \sum_{n \geq 0} s_n k_c^n(E)$$

Though there is no explicit way of linking these expansions (81) or (80) 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 equation (77) can be taken: one can provide a local set of coefficients $\{s_n\}_{V(E)}$ to expand the holomorphic part of the scattering matrix $\text{Hol}_U(E)$, and then calculate the scattering matrix from the Mittag-Leffler expansion (78).

An important question is that of the radius of convergence of the Mittag-Leffler expansion, in other terms how big can the vicinity $V(E)$ be? Humblet and Rosenfeld analyze this problem in section 1.4 of [2], and perform the Mittag-Leffler expansion (1.50). In the first paragraph of p.538 it is stated that Humblet demonstrated in his Ph.D. thesis that the Mittag-Leffler series will converge for $M \geq 1$ for $U(k)$, though this does not investigate the multi-channel case, and thus the multi-sheeted nature of the Riemann surface stemming from mapping (6). They assume at the beginning of section 10.2 that this property stands in the multi-channel 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 (c.f. theorem 0.2 p.139 of [63]). Though it is possible the Mittag-Leffler expansion might also hold separately on each sheet, in practice this requirement is however 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.

As we see, by performing the Mittag-Leffler expansion (78), we have traded-off a finite set of real, unwound, Wigner-Eisenbud parameters $\{E_{\lambda}, \gamma_{\lambda,c}\}$ that completely parametrized the energy dependence of the scattering matrix through (19), with an infinite set of complex Siegert-Humblet parameters $\{E_j, r_{j,c}\}$ and some local coefficients $\{s_n\}_{V(E)}$ for the holomorphic part — all of which are intricately intertwined through (55) which makes them dwell on a sub-manifold of the multi-sheeted Riemann surface of mapping (6). 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 poles and residues expansion (78). For computational purposes, this may be a trade-off worth doing.

IV. INVARIANCE WITH RESPECT TO CHANNEL RADIU

Section III provided new insights on the Wigner-Eisenbud, Brune, and Siegert-Humblet parametrizations of R-matrix theory with respect to their invariance to the arbitrary boundary condition $B_c$. As we saw, both the Brune and the Siegert-Humblet parameters are invariant under change of $B_c$, but not under change of channel radius $a_c$. This section is dedicated to invariance properties of R-matrix parameters to a change in channel radius $a_c$. This problem is both harder and 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 (c.f. eq. (2.29) and (2.31) sections III.2. p.27 of [64]), and a recent study of the limit case $a_c \rightarrow 0$ in [65]. We here focus on the Siegert-Humblet parameters $\{E_j, r_{j,c}\}$. Our main result of this section resides in theorem 4, which establishes a way of converting the Siegert-Humblet radioactive residue widths $\{r_{j,c}\}$ under a change of channel radius $a_c$.

Before introducing theorem 4, we bring forth the observation that the scattering matrix $U$ is invariant under change of channel radius $a_c$, i.e. for any channel $c$ we
have:
\[
\frac{\partial U}{\partial a_c} = 0 \quad (82)
\]

Since theorem 7 will show that the poles of the scattering matrix are exactly the ones of the Kapur-Peierls operator \( R_L \), which are the Siegert-Humblet poles \( \{ \varepsilon_j \} \), invariance (82) entails that the poles are invariant under change of channel radius \( a_c \), i.e.
\[
\frac{\partial \varepsilon_j}{\partial a_c} = 0 \quad (83)
\]

This is not the case for the other Siegert-Humblet parameters — the radioactive widths \( \{ r_{j,c} \} \). However, one can use invariance (82) to differentiate the scattering matrix \( U \) expression (19). Noticing in that process that definition (9) and the Bloch operator projection onto the channel surface, \( \rho_c = k_e a_c \), entail
\[
\frac{\partial \rho_c}{\partial a_c} = \frac{1}{a_c} \rho_c^2 O_e^{-1} \frac{1}{2} \left( \frac{1}{2} - L_c \right) \quad (84)
\]
this enables us to establish the following partial differential equations on the Kapur-Peierls matrix operator \( R_L \) elements: for the diagonal element,
\[
a_c \frac{\partial R_{Lc}}{\partial a_c} + (1 - 2Lc)R_{Lcc} - 1 = 0 \quad (85)
\]
and for off-diagonal ones,
\[
a_c \frac{\partial R_{Lcc'}}{\partial a_c} + \left( \frac{1}{2} - L_c \right) R_{Lcc'} = 0 \quad (86)
\]
which can be synthesized into expression,
\[
a \frac{\partial R_L}{\partial a} + \left( \frac{1}{2} \mathbb{1} - L \right) R_L + \mathbb{1} \circ \left[ \left( \frac{1}{2} \mathbb{1} - L \right) R_L - \mathbb{1} \right] = 0 \quad (87)
\]
where \( \circ \) designates the Hadamard matrix product, and where we used the notation:
\[
\left[ \frac{\partial R_L}{\partial a} \right]_{cc'} := \frac{\partial R_{Lcc'}}{\partial a_c} \quad (88)
\]
Equivalently, applying property (27) on partial differential equation (88) yields:
\[
a \frac{\partial R_L^{-1}}{\partial a} - R_L^{-1} \left( \frac{1}{2} \mathbb{1} - L \right) R_L - \mathbb{1} \circ \left[ R_L^{-1} \left( \frac{1}{2} \mathbb{1} - L \right) - R_L^{-1} \right] = 0 \quad (89)
\]

These first order partial differential equations are inconvenient to solve in that they are channel-dependent, and would thus give rise to equations for each cross term.

A. Radioactive width transformation under a change of channel radius

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 (17), one only requires the widths for each level of each channel, \( \gamma_j c \), and not some new parameter for each specific channel pair \( c, c' \) combination. In this spirit, we here demonstrate in theorem 4 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 4. Siegert-Humblet radioactive residue width \( r_{j,c} \) transformation under change of channel radius \( a_c \).

Invariance of the scattering matrix to channel radii \( a_c \) sets the following first-order linear partial differential equation on the radioactive widths \( \{ r_{j,c} \} \) of the Kapur-Peierls \( R_L \) operator residues,
\[
a_c \frac{\partial r_{j,c}}{\partial a_c} + \left( \frac{1}{2} - Lc \right) r_{j,c} = 0 \quad (90)
\]
which can be formally solved as,
\[
r_{j,c}(a_c) = r_{j,c}(a_c(0)) \sqrt{\frac{\alpha_c(0)}{\alpha_c}} \exp \left( \int_{a_c(0)}^{a_c} \frac{Lc(k_c x)}{x} dx \right) \quad (91)
\]
and explicitly integrates to:
\[
\frac{r_{j,c}(a_c)}{r_{j,c}(a_c(0))} = \frac{O_c(\rho_c(a_c(0)))}{O_c(\rho_c(a_c))} \sqrt{\frac{\alpha_c(0)}{\alpha_c}} \quad (92)
\]

**Proof.** Since we demonstrated the invariance (83), the Mittag-Leffler expansion (78) then entails that \( u_j \) from (79) satisfies invariance: \( \frac{\partial u_j}{\partial a_c} = 0 \). Applying result (84) to the latter then yields partial differential equation (90), the direct integration of which readily yields (91). Since \( L_c(\rho_c) := \frac{\rho_c}{\partial \rho_c} \frac{\partial \rho_c}{\partial \rho_c} \quad (93) \) integrates explicitly to (92). This result also stands for any degenerate state of multiplicity \( M_j \), where for each radioactive width \( r_{j,m} \) we have:
\[
\frac{r_{j,m}(a_c)}{r_{j,m}(a_c(0))} = \frac{O_c(\rho_c(a_c(0)))}{O_c(\rho_c(a_c))} \sqrt{\frac{\alpha_c(0)}{\alpha_c}} \quad (93)
\]

Note that for neutral particles (massive or massless) s-waves \( (\ell = 0) \), the outgoing wave function is \( O_c(\rho(\alpha_c)) = e^{ik_\alpha x} \) (c.f. table I), so that (92) yields \( r_{j,c}(a_c) = r_{j,c}(a_c(0)) \sqrt{\frac{\alpha_c(a_c(0))}{\alpha_c}} \). Alternatively, directly integrating (91) with the outgoing-wave reduced logarithmic derivative expression \( L_c(\rho(\alpha_c)) = ik_\alpha \alpha_c \) 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 wavenumbers \( k_c \in \mathbb{R} \), i.e. real energies above the channel threshold.
TABLE III. Roots \( \{\omega_n\} \) of the outgoing wave function \( O_\ell(r) \), algebraic solutions for neutral particles up to \( \ell \leq 4 \).

| \( \ell \) | \( \{\omega_n\} \) |
|---|---|
| 0 | \( \{0\} \) |
| 1 | \( \{-i\} \) |
| 2 | \( \{\frac{1}{2}(-\sqrt{3} - 3i), \frac{1}{2}(\sqrt{3} - 3i)\} \) |
| 3 | \( \{\omega_1^{(3)} \approx -1.75438 - 1.83891i, \omega_2^{(3)} \approx -2.32219i, \omega_3^{(3)} \approx 1.75438 - 1.83891i\} \) |
| 4 | \( \{\omega_1^{(4)} \approx -2.65742 - 2.10379i, \omega_2^{(4)} \approx -2.65742 - 2.10379i\} \) |

B. Elemental solutions through pole expansion

Having just established in theorem 4 the integral form (91), which integrates to (92) as a function of the outgoing wavefunction \( O_\ell(r) \), we here set-out in theorem 5 to express (91) as a function of the roots \( \{\omega_n\} \) of the outgoing wavefunction.

**Theorem 5.** ELEMENTAL POLE EXPANSION SOLUTION OF RADIOACTIVE RESIDUE \( r_{j,c} \) TRANSFORMATION UNDER CHANGE OF CHANNEL RADIUS \( a_c \).

Transformation (92) of Siegert-Humblet radioactive widths \( \{r_{j,c}\} \) under change of channel radius \( a_{(c)}^{(0)} \to a_{c} \), can be expressed elementally as:

\[
\frac{r_{j,c}(a_{c})}{r_{j,c}(a_{(c)}^{(0)})} = \sqrt{\frac{a_{c}}{a_{(c)}^{(0)}}} \left(\frac{a_{(c)}^{(0)}}{a_{c}}\right)^\ell e^{ik_c (a_c - a_{(c)}^{(0)})} \prod_{n \geq 1} \left(\frac{k_c a_c - \omega_n}{k_c a_{(c)}^{(0)} - \omega_n}\right)
\]

where \( \{\omega_n\} \) are the roots of the outgoing wave function \( \{\omega_n \mid O_\ell(\omega_n) = 0\} \).

In the Coulomb case, there are an infinite number of such roots \( \{\omega_n\} \).

For neutral particle channel \( c \) with angular momentum \( \ell \), there exists exactly \( \ell \) roots \( \{\omega_n\}_{n \in [1, \ell]} \), the exact and algebraically solvable values of which are reported in table III, up to angular momentum \( \ell = 4 \).

**Proof.** The proof is the element-wise integration, invoking Fubini's theorem to permute sum and integral, of (91) using the Mittag-Leffler pole expansion (13) of \( L_c(\rho) \), which we established in lemma 1. In the case of neutral particles there is a finite number of roots \( \{\omega_n\} \) so that the product in (94) is finite. Note that in the charged particles case, there is an infinity of roots \( \{\omega_n\} \), and the Weierstrass factorization theorem would thus usually require (94) to be cast in a Hadamard canonical representation with Weierstrass elementary factors. However, in (94), the product elements tend towards unity as \( n \) goes to infinity \( \left(\frac{k_c a_{(c)}^{(0)} - \omega_n}{k_c a_{(c)}^{(0)} - \omega_n}\right) \to 1 \), so that the infinite product in (94) should still converge. \( \square \)

Theorems 4 and 5 make explicit the behavior of the radioactive widths \( \{r_{j,c}\} \) under a change of channel radius \( a_{c} \). Strikingly, only the Kapur-Peierls matrix \( R_L \) appears in this change of variable. This means that the R-matrix \( R \) and the \( L^0 \) matrix function suffice to both compute the Siegert-Humblet parameters \( \{E_{ij}, r_{j,c}\} \) from (55), and to change the radioactive widths \( \{r_{j,c}\} \) under a change of channel radius \( a_{c} \). This novel result portrays the Siegert-Humblet parameters as allowing a simple energy dependence to the scattering matrix (78) — albeit locally and needing the expansion coefficients (80) — all the while being boundary condition \( B_c \) independent and easy to transform under a change of channel radius \( a_{c} \).
V. CONTINUING THE SCATTERING MATRIX TO COMPLEX ENERGIES WHILE CLOSING CHANNELS BELOW THRESHOLDS

In section 5.2 of [2], Humblet and Rosenfeld continue the scattering matrix to complex wavenumbers \( k_c \in \mathbb{C} \), and define corresponding open and closed channels. They however 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 & Thomas, where they explicitly annul the elements of the scattering matrix below thresholds, as stated in the paragraph between equations (2.1) and (2.2) of section VII.1. p.289 [5]. Claude Bloch ingeniously circumvents the problem by explicitly stating after eq. (50) in [13] 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.

Echoing section III B 2, we dedicate this section to this question of how to extend the scattering matrix to complex wavenumbers \( k_c \in \mathbb{C} \), while closing the channels below threshold.

A. Forcing sub-threshold elements to zero: the legacy of Lane & Thomas

To close the channels for real energies below threshold, the simplest approach is the one proposed by Lane & Thomas in [5]. This approach exploits the ambiguity, discussed in section III B 2, when it comes to defining the shift \( S(E) \) and penetration \( P(E) \) factors for complex energies \( E \in \mathbb{C} \). With decomposition (28), the scattering matrix expressions (19) can be re-written, for real energies above threshold, according to section VII.1. equation (1.6b) in [5]:

\[
U = \Omega \left( I + \omega \mathfrak{P}^{1/2} R_L \mathfrak{P}^{1/2} \right) \Omega \tag{95}
\]

with the values defined for energies above the thresholds in III.3.a. p.271 of [5]:

\[
\Omega = O^{-1} I \\
\mathfrak{P} = \rho O^{-1} I^{-1} \tag{96}
\]

Let us note that the Mittag-Leffler expansion (54) of the Kapur-Peierls matrix \( R_L \) operator can still be performed.

Lane & Thomas do not specify how they would continue the quantities (96) for negative energies, as they state “we need not be concerned with stating similar relations for the negative energy channels” (c.f. paragraph after equation (4.7c), p.271.). but they do specify that \( P = 0 \) below threshold energies and \( P = \mathfrak{P} \) above. This means that plugging-in \( P \) in place of \( \mathfrak{P} \) in (96) 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 equation (1.10) in [5] VIII.1. p.291. Note that this approach only annuls the off-diagonal terms of the scattering cross section, leaving non-zero cross sections for the diagonal \( \sigma_{cc}(E) \), even below threshold. Indeed, equation (4.5a) section III.4.a., p.271 of [5] gives \( \Omega_c = e^{i(\omega - \phi_c)} \), whilst the cross section is gotten by the amplitudes of the transmission matrix \( T(E) \), defined as \( T_{cc'} := \delta_{cc'} e^{2i\phi_{c'}} - U_{cc'} \) in (2.3), section VIII.2. p.292. For sub-threshold real energies, the diagonal term of the transmission matrix is thus equal to \( T_{cc} = e^{2i\phi_c} (1 - e^{-2i\phi_c}) \). This means that in the Lane & Thomas approach, all channels \( c' \neq c \) are force-closed to zero below the incoming channel threshold \( E < E_{T_c} \), except for the \( c \rightarrow c \) reaction, which is pudiqely overlooked as non-physical.

Of course, this approach comes at the cost of sacrificing the analytic properties of the scattering matrix \( U \): since \( P_c = \Im \{L_c\} \), the penetration factor is no longer meromorphic and thus neither is \( U \), going directly against a vast amount of literature on the analytic properties of the scattering matrix [2, 3, 14–21, 55, 63, 66, 67]. This is the approach presently taken by the SAMMY code at Oak Ridge National Laboratory [68], and upon which thus rest numerous ENDF evaluations [1].

We would like to note that under careful reading, this might not actually have been the approach intended by Lane & Thomas in [5]. Indeed, Lane & Thomas never specify how to prolong the \( \mathfrak{P} \) to subthreshold energies, and in equation (95) it is \( \mathfrak{P} \) that is present and not \( P \). They do however note in the paragraph between equations (2.1) and (2.2) of section VII.1. p.289, that “as there are no physical situations in which the \( I^- \) 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 \( O^- \) and \( I^- \) 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 allow to keep the analytic properties of the scattering matrix, with \( \mathfrak{P} := \rho O^{-1} I^{-1} \) still analytically continued, albeit at the cost of not knowing when in the complex plane should the Wronskian \( w_c \) be set to zero — perhaps only on \( \mathbb{R}_- \), which would then become a branch line.

As we will show in theorem 6 of section VB, as long as the scattering matrix is continued so as to keep the Wronskian relation (7) intact, the poles of the outgoing scattering wave function \( O_c \) cancel out of the scattering expressions (19) and (95). The Wronskian condition (7) is conserved when keeping \( \mathfrak{P} \) from (96) — instead of the definition \( P_c := \Im \{L_c\} \), which cannot respect the
In section II B, the incoming Wronskian relation (7) — 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 & Thomas approach, an entire field of physics and mathematics has studied the analytic continuation of the scattering matrix to complex wavenumbers \( k_c \in \mathbb{C} \) [2, 14–20, 63, 67, 69–71].

As we saw, there is no ambiguity as to how to continue the \( L^0 \) matrix function, and thus the Kapur-Perelis matrix \( R_L \), to complex wave numbers. Indeed, as discussed in section II B, the incoming \( I_c(\rho_c) \) and outgoing \( O_c(\rho_c) \) wave functions can be analytically continued to complex wavenumbers \( k_c \in \mathbb{C} \), and through the multi-sheeted mapping (6) to complex energies \( E \in \mathbb{C} \). This naturally yields the meromorphic continuation of the scattering matrix to complex energies (78).

The shortcoming of this analytic continuation approach is that it cannot annul the channel elements of the scattering matrix for sub-threshold energies \( E < E_{T_c} \). Indeed, analytic continuation (78) means the scattering matrix \( U \) is a meromorphic operator from \( \mathbb{C} \) to \( \mathbb{C} \) on the multi-sheeted Riemann surface of mapping (6). 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 definition (39), legacy of Lane & Thomas, when computing the scattering matrix in equation (19). This has been the subject of an ongoing controversy in the field on how to continue the scattering matrix to complex wave numbers.

This article argues that analytic continuation (42) is the physically correct way of continuing the scattering matrix to complex energies. To support this, we advance and demonstrate three new arguments: analytic continuation cancels out spurious poles otherwise introduced by the outgoing wave functions \( O_c \) (theorem 6); analytic continuation respects generalized unitarity (theorem 8); and, for massive particles, analytic continuation of real wavenumber expressions to sub-threshold energies naturally sees the transmission matrix evanesc on the physical sheet (theorem 9), while always closing the channels by annulling the cross section (theorem 10).

### C. Spurious poles cancellation for analytically continued scattering matrix

We here show that the outgoing-wave \( O \) a priori introduces spurious poles to the scattering matrix \( U \); but show how these are cancelled out if the R-matrix \( R \), the wavefunctions \( O, I \), and thus the \( L^0 \) matrix function, are analytically continued to complex wavenumbers, while maintaining a constant Wronskian (7).

#### 1. Assuming semi-simplicity of poles in R-matrix theory

Let us first start with a note on high-order poles. 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 resolvent at a pole value; c) Geometric multiplicity: the dimension of the associated nullspace.

From equation (53) 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 equation (53), the residues might be rank-\( M_j \), but the Laurent order is still unity (no \( \frac{1}{(E - E_j)^k} \) 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 \( n_1, ..., n_{m_a} \), then the geometric multiplicity is equal to \( m_g \), the algebraic multiplicity \( m_a \) is the sum \( m_a = n_1 + ... + n_{m_a} \), and the Laurent order is the maximum \( \max \{ n_1, ..., n_{m_a} \} \).

Alternatively, these can be defined as follows: Let \( M(z) \) be a complex symmetric meromorphic matrix operator, with a root at \( z = z_0 \) (i.e. \( M(z_0) \) is non-invertible). 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 \( \frac{d^m}{dz^m} \det (M(z)) \bigg|_{z=z_0} = 0 \); alternatively, using Cauchy’s theorem, the first integer \( m_a \) such that \( \oint_{C_{z_0}} \frac{M(z)}{(z-z_0)^{m_a}} \, dz = 0 \). The geometric multiplicity \( m_g \) is the dimension of the kernel (nullspace), i.e. \( m_g = \dim (\text{Ker} (M(z_0))) \). In general the algebraic multiplicity is greater than the geometric one: \( m_a \geq m_g \).

\( M(z_0) \) is said to be semi-simple if its geometric and algebraic multiplicities are equal, i.e. \( m_a = m_g \) (c.f. theorem 2, p.120 in [72]). Semi-simplicity can be established using the following result: \( M(z_0) \) is semi-simple if, and only if, for each nonzero \( v \in \text{Ker} (M(z_0)) \), there exists \( w \in \text{Ker} (M(z_0)) \) such that:

\[
\left( \frac{dM}{dz} \right)_{z=z_0} w \neq 0
\]  

(97)

If an operator \( M(z_0) \) is semi-simple at a root \( z_0 \), then...
\( z_0 \) is a pole of Laurent-order one for the inverse operator 
\[ M^{-1}(z) \sim \frac{M}{v(z)} \]  
For Hermitian operators, the semi-simplicity property is guaranteed. However, resonances seldom correspond to Hermitian operators. In our case, the resonances correspond to the poles of the scattering matrix \( U(E) \), which is not self-adjoint but complex symmetric \( U^T = U \) (c.f. equation (2.15) section VI.2.c p.287 in \cite{5}). For complex symmetric operators, semi-simplicity is not guaranteed in general, even when discarding the complex case of quasi-null 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 semi-simple scattering matrices, and the Laurent development order of the resonance poles can be higher. For instance, we can devise examples of non-semi-simple inverse level matrices from definition (18) 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 semi-simplicity is broken is a hyper-plane of the space of R-matrix parameters. This gives credit to the traditional physics arguments that the probability of this occurring is quasimult: 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 chapter 4 “Black Box Scattering in \( \mathbb{R}^n \)” of \cite{67}, in particular theorem 4.4 (Meromorphic continuation for black box Hamiltonians), theorem 4.5 (Spectrum of black box Hamiltonians), theorem 4.7 (Singular part of \( RV(\lambda) \) for black box Hamiltonians), and theorem 4.39 (Generic simplicity of resonances for higher dimensional black box with potential perturbation). In other terms, we assume semi-simplicity is almost always guaranteed through R-matrix parametrizations.

Henceforth, we use this argument to continue assuming the Kapur-Parleis matrix \( R_L \) is usually semi-simple, and thus the Laurent order of the radioactive poles \( \{E_j\} \) in (53) is, in practice, one.

But let us be aware that in general scattering theory, the scattering operator may exhibit high-order poles \cite{63,67,73}, and efforts are being made to have these “exceptional points” of second order arise in the specific case of nuclear interactions \cite{74,75}. The traditional R-matrix assumption where the poles of the scattering matrix are almost-always of Laurent-order one is unable to describe these physical phenomena.

2. Outgoing wave \( O \) introduces spurious poles

We have given reasons to assume that the poles of the Kapur-Parleis matrix \( R_L \) are simple (i.e. or Laurent order one), however, looking at (19) shows that the roots of the outgoing wave functions \( O \) could endow the scattering matrix with additional poles, through \( O^{-1} \), and that these poles could potentially have higher Laurent orders, since \( O^{-1} \) appears twice in expression (19).

We have established through Lemma 5 that \( O^{-1} \) is semi-simple because it is diagonal with simple roots. This result will be used in theorem 6 to show that these poles cancel out of the scattering matrix if the Wronskian condition (7) is maintained.

**Lemma 5. Diagonal Semi-Simplicity** - If a diagonal matrix \( D^{-1}(z) \) is composed of elements with simple roots \( \{\omega_k\} \), then its inverse is semi-simple, i.e. when a pole \( \omega_k \) of a diagonal matrix \( D(z) \) has an algebraic multiplicity \( M_k > 1 \) the Laurent development order of the pole remains 1 while the associated residue matrix is of rank \( M_k \), and can be expressed as:

\[
D(z) = \frac{D_k}{z-\omega_k} \quad (98)
\]

with

\[
D_k = \sum_{m=1}^{M_k} v_k v_k^T D_0^{-1}(1) v_k \quad (99)
\]

**Proof.** Without loss of generality, a change of variables can be performed so as to set \( \omega_k = 0 \).

Let \( D(z) = \text{diag} (d_1(z), d_2(z), \ldots, d_1(z), d_j(z), d_n(z)) \) be a diagonal meromorphic complex-valued operator, which admits a pole at \( z = 0 \). \( D^{-1}(z) = \text{diag} (d^{-1}_1(z), d^{-1}_2(z), \ldots, d^{-1}_1(z), d^{-1}_j(z), d^{-1}_n(z)) \) is well known, and det \( (D^{-1})(z=0) = d^{-1}_1(z)^2 \prod_{j \neq 1} d^{-1}_j(z) \). Let us assume only \( d^{-1}_1(z) = 0 \), with a simple root, so that \( d_1(z) = d_0 + \frac{R_1}{z} \). Then det \( (D^{-1})(z) = 0 = d^{-1}_1(z)^2 \prod_{j \neq 1} d^{-1}_j(z) \) has a double root: the algebraic multiplicity is thus 2. However, it is immediate to notice that:

\[
D(z) = \frac{\text{diag} (d_1(z), d_2(z), \ldots, d_1(z), d_j(z), d_n(z))}{v(z=0)} = \text{diag} (d_0, d_2(z), \ldots, d_0(z), d_j(z), d_n(z))
\]

\[
+ \frac{1}{z} \text{diag} (R_1, 0, \ldots, R_1, 0, 0)
\]

This means the Laurent development order remains 1, albeit the algebraic multiplicity of the pole is 2 (or higher \( M_k \)). Thus, it can be written that:

\[
D(z) = \frac{D_0}{v(z=0)} + \frac{D_1}{z}
\]

When solving for the non-linear Eigenproblem

\[
D^{-1}(z)v = 0
\]

the kernel is no longer an eigenline, but instead spans \( \{v_1, v_2\} \):

\[
\text{Ker} (D_0^{-1}) = \text{span} (v_1, v_2)
\]
with \( \mathbf{v}_1 = a_1 [1, 0, \ldots, 0, 0]^T \) and \( \mathbf{v}_2 = a_2 [0, 0, \ldots, 1, 0]^T \). Then, following Gohberg-Sigal’s theory [59], the fundamental property:

\[
D^{-1} D = I
\]

and the Laurent development around the pole:

\[
D^{-1}(z) = \frac{D_0^{-1} + zD^{-1}(1) + O(z^2)}{v(z=0)}
\]

yield the relations:

\[
D_0^{-1}D_0 + D^{-1}(1)D_1 = \mathbb{I}
\]

\[
D_0^{-1}D_1 = 0
\]

Constructing \( D_1 \) to satisfy the latter then entails

\[
D_1 = \frac{v_1 v_1^T}{v_1^T D_0^{-1}(1) v_1} + \frac{v_2 v_2^T}{v_2^T D_0^{-1}(1) v_2}
\]

where the transpose is used because the matrix is complex symmetric. This reasoning immediately generalizes to expression (99).

Let \( \{\omega_k\} \) be all the roots of the outgoing-wave functions (i.e. the poles of inverse outgoing wave \( O^{-1} \)), which we can find by solving the non-linear Eigenvalue problem:

\[
O(\omega_k)w_{km} = 0 \tag{100}
\]

Since \( O^{-1} \) is diagonal, Lemma 5 entails it is semi-simple: the algebraic multiplicities are equal to the geometric multiplicities, and thus the poles \( \{\omega_k\} \) all have Laurent-order one.

Situations can arise where same-charge channels within the same total angular momentum \( J^* \) will carry same angular momenta \( \ell_c = \ell_c \) and equal channel radii \( a_c = a_c \). In that case, the geometric multiplicity \( M_k \) of pole \( \omega_k \) will be equal to the number of channels sharing the same functional outgoing waves \( O_c = O_c \). Diagonal semi-simplicity Lemma 5 then establishes that the residue of \( O^{-1} \) associated to pole \( \omega_k \) is now a diagonal rank-\( M_k \) matrix, \( \mathbf{D}_k \), expressed as:

\[
\mathbf{D}_k = \sum_{m=1}^{M_k} \frac{W_{km} W_{km}^T}{W_{km}^T O^{(1)}(\omega_k) W_{km}} \tag{101}
\]

where \( O^{(1)}(\omega_k) \) designates the first derivative of \( O \), evaluated at the pole value \( \omega_k \). This establishes the existence of higher-rank residues associated to the inverse outgoing wave function \( O^{-1} \).

Notice that if the channel radii \( \{a_c\} \) where 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 means that in practice these high-rank residues are legion.

3. Poles from the outgoing waves \( O \) cancel out of the analytically continued scattering matrix \( \mathbf{U} \)

We just established that the poles \( \{\omega_k\} \) of the inverse outgoing wave \( O^{-1} \) had Laurent-order one, potentially with higher-rank residues (101). At first sight, (19) seems to entail these \( \{\omega_k\} \) poles should also be poles of the scattering matrix \( \mathbf{U} \), possibly with Laurent order two. We here establish with theorem 6 that if the Wronskian condition (7) is satisfied through analytic continuation, the \( \{\omega_k\} \) poles cancel out of the scattering matrix \( \mathbf{U} \), leaving only the poles \( \{\xi_j\} \) of the Kapur-Peierls matrix \( \mathbf{R}_L \) as the scattering poles.

**Theorem 6. Analytic continuation of scattering matrix cancels spurious poles.**

If the Wronskian condition (7) is satisfied through analytic continuation of the Kapur-Peierls operator \( \mathbf{R}_L \) and the wavefunctions \( \mathbf{I} \) and \( \mathbf{O} \), then the poles \( \{\omega_k\} \) of the inverse outgoing wave \( O^{-1} \) cancel out of the scattering matrix \( \mathbf{U} \) in equation (19).

**Proof.** Consider the scattering matrix expression \( \mathbf{U} = O^{-1}[I + 2i\rho^{1/2}R_L O^{-1}\rho^{1/2}] \) from (19). Result (101) entails that, in the vicinity of \( \omega_k \), root of the outgoing wave-function \( O \), the residue is locally given by:

\[
\mathbf{U}(z) = \mathbf{U}_0(\omega_k) + \frac{\mathbf{D}_k [I + 2i\rho^{1/2}R_L O^{-1}\rho^{1/2}]_{E=\omega_k}}{E-\omega_k} \tag{102}
\]

We now notice that evaluating the Kapur-Peierls \( \mathbf{R}_L \) operator (20) at the pole value \( \omega_k \) yields the following equality:

\[
R_L O^{-1}(\omega_k) w_{km} = -[\rho O^{(1)}]^{-1}(\omega_k) w_{km} \tag{103}
\]

Plugging (103) into the residue of (102), and using the fact that (101) guarantees \( \mathbf{D}_k \) is a linear combination of \( w_{km} w_{km}^T \), we then have the following equality on the residues at poles \( \omega_k \):

\[
\mathbf{D}_k [I + 2i\rho^{1/2}R_L O^{-1}\rho^{1/2}]_{E=\omega_k} = \mathbf{D}_k [I - 2iO^{(1)}]^{-1}_{E=\omega_k} \tag{104}
\]

The rightmost term is diagonal and independent from the resonance parameters. Since the Wronskian matrix \( \mathbf{w} \) of the external region interaction (for Coulomb or free particles) is constant, \( \mathbf{w} = O^{(1)} \mathbf{I} - \mathbf{I}^{(1)} \mathbf{O} = 2\mathbb{I} \), evaluating at outgoing wave-function root \( \omega_k \), one finds \( 2\mathbb{I} = O^{(1)} \mathbf{I}(\omega_k) \). Plugging this result into (104) annuls the corresponding residue from the scattering matrix, i.e.:

\[
\mathbf{D}_k [I + 2i\rho^{1/2}R_L O^{-1}\rho^{1/2}]_{E=\omega_k} = 0 \tag{105}
\]

Thus, if the Wronskian condition (7) is respected, the \( \{\omega_k\} \) poles cancel out of the scattering matrix \( \mathbf{U} \).
wave functions and maintain a constant Wronskian (7), without which the \( \{ \omega_k \} \) poles would not cancel from the scattering matrix \( \bar{U} \).

Finally, theorem 7 is a direct corollary of theorem 6, and having assumed the poles of the Kapur-Peierls operator almost always be of Laurent order one:

**Theorem 7.** In R-matrix theory the Scattering matrix poles are the Kapur-Peierls radioactive poles.

In the context of the R-matrix scattering model, when the scattering matrix \( U \) is analytically continued to complex energies \( E \in \mathbb{C} \) such as to respect the Wronskian condition (7), the poles of the scattering matrix \( U \) are exactly the poles of the Kapur-Peierls operator \( R_L \), i.e. the Siegert-Hamilton poles \( \{ \epsilon_j \} \) from (55) and (56). These poles are almost always of Laurent-order of one.

Importantly, both the Lane & Thomas force-closing of sub-threshold channels V A or the analytic continuation V B will yield the same cross section values for real energies above thresholds. However, we here demonstrated that the choice of analytic continuation in equation (19), respecting the Wronskian condition (7), leads to the cancellation from the scattering matrix \( U \) of the \( \{ \omega_k \} \) 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 \( \Phi = P \) been made in equation (95), as discussed in section V A. Indeed, choosing definition (39), i.e. \( P = \Re \{ L(z) \} \in \mathbb{R} \), will fail to cancel out the \( \{ \omega_k \} \) poles. Conversely, defining the penetration by analytic continuation (41) as \( P(z) = \frac{1}{2} \left( L(z) - [L(z)]^* \right) \in \mathbb{C} \) will guarantee the cancellation of the \( \{ \omega_k \} \) poles from the scattering matrix \( U \) if using (95). Notice this is almost the definition (111) of \( \Delta L(\rho) \) we hereafter use in the proof of the generalized unitarity. Then, to force-close sub-threshold channels, one could set the Wronskian to zero, as proposed by Lane & Thomas in the paragraph between equation (2.1) and (2.2) of section VII.1. p.289.

This shifts the problem to how to maintain the Wronskian condition (7) while setting the Wronskian to zero, as proposed by Lane & Thomas in the paragraph between equation (2.1) and (2.2) of section VII.1. p.289. This is also consistent with approaches other than R-matrix to modeling nuclear interactions (c.f. commentary above eq. (3) p.4 in [75], [71], or [69]).

We now show that analytically continuing the R-matrix expression (19) ensures the scattering matrix respects Eden & Taylor generalized unitarity condition.

**Theorem 8.** Analytic continuation of the R-matrix expression for the scattering matrix ensures generalized unitarity.

By performing the analytic continuation of the R-matrix expression (19), the scattering matrix \( \bar{U} \) satisfies Eden & Taylor’s generalized unitarity condition (107).

**Proof.** The proof is based on the conjugacy relations of the outgoing and incoming wavefunctions eq. (2.12), VI.2.c. in [5], whereby, for any channel \( c \):

\[
\begin{align*}
\left[ O_c(k_c^*) \right]^* &= I_c(k_c), & \left[ I_c(k_c^*) \right]^* &= O_c(k_c), \\
O_c(-k_c) &= I_c(k_c), & I_c(-k_c) &= O_c(k_c), \\
-O_c(k_c^*)^* &= I_c^*(k_c^*), & -I_c^*(k_c^*) &= O_c^*(k_c^*)
\end{align*}
\]

(108)

where the third line was obtained by taking the derivative of the second. Recalling the definition of the outgoing-wave reduced logarithmic derivative (9), these conjugacy relations (108) entail the following on \( L \):

\[
\begin{align*}
\left[ L_c(k_c^*) \right]^* &= L_c(-k_c), & \left[ L_c(-k_c^*) \right]^* &= L_c(k_c)
\end{align*}
\]

(109)

We also notice that the Wronskian condition (7) is equivalent to:

\[
2i\rho_c \frac{\partial O_c}{\partial I_c} = \rho_c \left[ \frac{O_c^{*}(1)}{O_c} - \frac{I_c^{*}(1)}{I_c} \right]
\]

(110)
one recognizes here the definition (9) of $L$, and, using the conjugacy relations (109), the Wronskian condition (110) can be expressed as a difference of the reduced logarithmic $L_c$ derivatives as:

$$\Delta L_c(k_c) := L_c(k_c) - L_c(-k_c) = \frac{2i\rho_c}{O T_e}(k_c)$$  \hspace{1cm} (111)

Defining the diagonal matrix $\Delta L := \text{diag}(\Delta L_c(k_c))$, we can then re-write, similarly to (95), the R-matrix expression (19) of the scattering matrix $U$ as a function of $\Delta L_c(k_c)$, so that:

$$U = O^{-1} \left[ I + \left[ \rho^{1/2} R_L \rho^{-1/2} \right] \Delta L \right] I$$

$$= I \left[ I + \Delta L \left[ \rho^{-1/2} R_L \rho^{1/2} \right] \right] O^{-1}$$  \hspace{1cm} (112)

Notice again how this expression is closely related to the analytic continuation of expression (95).

Coming back to the Eden & Taylor continuation (106), let us now establish a relation between the Kapur-Peierls operator $R_L$ and $\Delta L$. From the definition (20) of the Kapur-Peierls operator $R_L$, recalling that under Eden & Taylor continuations (106) the energy $E$ from mapping 6 remains unaltered, and given that the boundary-condition $B_c$ in the $L^0$ matrix function is real and thus the R-matrix parameters (17) are too, it follows that:

$$\left[ R_L^{-1}(k) \right]^* \cdot R_L^{-1}(k) = \left[ \Delta L(k) \right]$$  \hspace{1cm} (113)

where we have used the $L$ conjugacy relations (109) to establish that all channels $c \notin \tilde{C}$ cancel out, and the rest yield $\Delta L_{c \in \tilde{C}}(k_c)$. The $\Delta L$ thus designates the sub-matrix composed of all the channels $c \in \tilde{C}$. Multiplying both left and right, and considering the sub-matrices on the channels $c \in \tilde{C}$ thus yields:

$$\hat{R}_L(k) - \left[ \hat{R}_L(k) \right]^* = \hat{R}_L(k) \Delta L(k) \left[ \hat{R}_L(k) \right]^*$$  \hspace{1cm} (114)

This relation is what guarantees the scattering matrix $U$ satisfies generalized unitarity condition (107). Indeed, let us develop the left-hand side of (107), using expressions (112) on the sub-matrices of the channels $c \in \tilde{C}$:

$$\hat{U}(k) \left[ \hat{U}(k) \right]^* = \hat{O}^{-1}(k) \left[ I + \left[ \rho^{1/2} R_L \rho^{-1/2} \right](k) \Delta L(k) \right] \hat{I}(k)$$

$$\times \left[ \hat{I}(k) \left[ I + \Delta L(k) \left[ \rho^{-1/2} R_L \rho^{1/2} \right](k) \right] \hat{O}^{-1}(k) \right]^*$$

$$= \hat{O}^{-1}(k) \left[ I + \left[ \rho^{1/2} R_L \rho^{-1/2} \right](k) \Delta L(k) \right] \hat{I}(k) \times$$

$$\left[ \hat{O}^{-1}(k^*) \right]^* \left[ I + \left[ \rho^{-1/2} R_L \rho^{1/2} \right](k^*) \left[ \Delta L(k^*) \right]^* \right] \left[ \hat{I}(k^*) \right]^*$$  \hspace{1cm} (115)

Noticing that conjugacy relation (109) entail the following $\Delta L$ symmetry from definition (111), $\left[ \Delta L(k^*) \right]^* = -\Delta L(k)$, and making use of the conjugacy relations for the wave functions (108), we can further simplify (115) to:

$$\hat{U}(k) \left[ \hat{U}(k) \right]^* = I$$

$$+ \hat{O}^{-1}(k) \left[ \rho^{1/2} R_L \rho^{-1/2} \right](k) \times$$

$$\left[ \left[ \rho^{1/2} R_L \rho^{-1/2} \right]^{-1}(k^*) \right]^* - \left[ \rho^{1/2} R_L \rho^{-1/2} \right]^{-1}(k) - \Delta L(k)$$

$$\times \left[ \left[ \rho^{-1/2} R_L \rho^{1/2} \right](k^*) \right]^* \Delta L(k) \hat{O}(k)$$  \hspace{1cm} (116)

In the middle we recognize identity (113), where the $\rho^{1/2}$ cancel out by commuting in the diagonal matrix identity (113). Property (113) thus annuls all non-identity terms, leaving Eden & Taylor’s generalized unitarity condition (107) satisfied.

Let us also note that the proof required real boundary conditions $B_c \in \mathbb{R}$. Thus, in R-matrix parametrization (19), real boundary conditions $B_c \in \mathbb{R}$ are necessary for the scattering matrix $U$ be unitarity (and by extension generalized unitary).

Theorem 8 beholds 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 wavenumbers $k_c \in \mathbb{C}$.

E. Closure of sub-threshold cross sections through analytic continuation

We finish this article with the key question of how to close sub-threshold 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 mappings (2) or (4), adequate definitions and careful consideration will both make the transmission matrix evanescent sub-threshold (in a classical case of quantum tunnelling), and annul the sub-threshold cross-section — the physically measurable quantity.

The equations linking the scattering matrix $U$ to the cross section — equations (1.9), (1.10) and (2.4) section VIII.1. of [5] pp.291-293 — were only derived for real positive wavenumbers. Yet, when performing analytic continuation of them to sub-threshold energies, the quantum tunneling effect will naturally make the transmission matrix infinitesimal on the physical sheet of mapping (2). Indeed, the transmission matrix, $T$, is defined in [5] after
eq. (2.3), VIII.2. p.292, as:
\[ T_{cc} := \delta_{cc} e^{2i\omega_c} - U_{cc} \] (117)
where \( \omega_c \) is defined by Lane & Thomas in eq.(2.13c) III.2.b. p.269, and used in eq.(4.5a) III.4.a. p.271 in [5], and is the difference \( \omega_c = \sigma_{\ell c}(\eta_c) - \sigma_{c}(\eta_c) \), where the Coulomb phase shift, \( \sigma_{\ell c}(\eta_c) \) is defined by Ian Thompson in eq.(33.2.10) of [29]. Defining the diagonal matrix \( \mathbf{\omega} := \text{diag}(\omega_c) \), and using the R-matrix expression (19) for the scattering matrix, the Lane & Thomas transmission matrix (117) can be expressed with R-matrix parameters as:
\[ T_{L&T} := -2iO^{-1} \left[ \begin{array}{c} I - O e^{2i\omega} \\
2i \end{array} \right] + \rho^{1/2} R_{L} O^{-1/2} \rho^{1/2} \] (118)
The angle-integrated partial cross sections \( \sigma_{cc}(E) \) can then be expressed as eq.(3.2d) VIII.3. p.293 of [5]:
\[ \sigma_{cc}(E) = 4\pi g_{J_2} \left| \frac{1}{O_{k_e}} \right|^2 \left( \Theta + \rho^{1/2} R_{L} O^{-1/2} \rho^{1/2} \right)^2 \] (119)
where \( g_{J_2} := \frac{2J_2+1}{(2J_2+1)(2J_2+3)} \) is the spin statistical factor defined eq.(3.2c) VIII.3. p.293. Plugging-in the transmission matrix R-matrix parametrization (118) into cross-section expression (119) then yields: [5]:
\[ \sigma_{cc} = 4\pi g_{J_2} \left| \frac{1}{O_{k_e}} \right|^2 \left( \Theta + \rho^{1/2} R_{L} O^{-1/2} \rho^{1/2} \right)^2 \] (120)
An alternative, more numerically stable, way of computing the cross section is used at Los Alamos National Laboratory, where one of us, G. Hale, introduced the following rotated transmission matrix, defined as:
\[ T_{H} := -e^{-i\omega T_{L&T}}e^{-i\omega} \] (121)
and whose R-matrix parametrization is thus
\[ T_{H} = H_{L}^{-1} \left[ \rho^{1/2} R_{L} \rho^{1/2} H_{L}^{-1} - \left( \frac{H_{L} - H_{c}}{2i} \right) \right] \] (122)
where \( H_{L} \) are defined as in eq.(2.13a)-(2.13b) III.2.b p.269 [5]:
\[ H_{L} = O_{e} e^{i\omega} = G_{c} + iF_{c} \]
\[ H_{c} = L_{e} e^{-i\omega} = G_{c} - iF_{c} \] (123)
and for which we refer to Ian. J. Thompson's Chapter 33, eq.(33.2.11) in [29], or Abramowitz & Stegun chapter 14, p.537 [28]. The partial cross section is then directly related to the \( T_{H} \) rotated transmission matrix (121) as:
\[ \sigma_{cc}(E) = 4\pi g_{J_2} \left| k_{c}(E) \right|^2 \] (124)

**Theorem 9.** EVANESCENT OF SUB-THRESHOLD TRANSMISSION MATRIX.
For massive particles, analytic continuation of R-matrix parametrization (19) makes the sub-threshold transmission matrix \( T \), defined as (118), evanescent on the physical sheets of mappings (2), or (4). In turn, this quantum tunnelling entails the partial cross sections \( \sigma_{cc}(E) \) become infinitesimal below threshold.

**Proof.** The proof is based on noticing that both transmission matrix expressions (118) and (121) entail their modulus square is proportional to:
\[ |T_{cc}|^2(E) \propto \left| \frac{1}{H_{c}(E)} \right|^2 \] (125)
This is because \( R_{L} O^{-1} = \left[ O \left[ R^{-1} - B \right] - \rho O^{(1)} \right]^{-1} \), which does not diverge below threshold. Asymptotic expressions for the behavior of \( H_{c}(\rho) \) then yield, for small \( \rho \) values:
\[ H_{c}(\rho) \sim \rho^{-\ell} \left( \frac{\rho}{(2\ell + 1)C_{\ell}(\eta)} \right) - iC_{\ell}(\eta) \rho^{\ell + 1} \] (126)
and asymptotic large-\( \rho \) behavior:
\[ H_{c}(\rho) \sim e^{i(\rho - \eta \ln(2\rho) - \frac{1}{2} \ell \pi + \sigma_{\ell}(\eta))} \] (127)

Above the threshold, \( \rho \in \mathbb{R} \) is real and thus equation (127) shows how \( |H_{c}(\rho)| \) will now tend to a 1\( \rightarrow 1 \). In other terms, the \( \rho \) term cancels out of the cross section expressions (120) and (124) for open-channels above threshold. Yet, from mappings (2) and (4), the sub-threshold dimensionless wavenumber is purely imaginary: \( \rho \in \mathbb{R} \). Since asymptotic form (127) is dominated in modulus by: \( |H_{c}(\rho)| \sim e^{i\rho} \). Depending on which sheet \( \rho \) is continued sub-threshold, we can have \( \rho = \pm i\pi \), with \( \pi \in \mathbb{R} \). Thus, on the non-physical sheet \( \{ E, \ldots, cE \} \) for the given channel \( c \) of \( \rho_{c} \), the transmission matrix (125) experiences exponential decay of \( 1/|H_{c}(\rho)| \) leading to the evanescence of the cross section (119), or (124). In effect, this means that the \( |O_{c}(\rho_{c})| \) term in (120) 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 \( |E - E_{T}| \). This is a classical evanescence behavior of quantum tunneling.

What happens when continuing on the physical sheet \( \{ E, \ldots, cE \} \), as \( |H_{c}(\rho)| \) will now tend to a 1\( \rightarrow 1 \) version? 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, evanescence result ought to also stand, despite the apparent divergence.

Note that for photon channels, the semi-classic mapping (3) does 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 by closing the cross sections below threshold. At distance $r_c$ from the center of mass of the nucleus, and at wavenumber $k_c$, distant from the threshold as $|E - E_{T_c}|$, the asymptotic behavior or the cross-section below threshold is:

$$\ln \left( \sigma_{cc'}(k_c, r_c) \right) \sim -2r_c|k_c| \quad \text{for} \quad E_c \leq E_{T_c}$$  \hspace{1cm} (128)

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 $^{238}\text{U}$ target reacting with neutron $n$ channel, evanesence (128) would be of the rate of $\log_{10} \left( \sigma_{cc'}(k_c, r_c) \right) \sim -3 \times 10^{16} r_c \text{eV} \sqrt{\Delta E_c \text{eV}}$. For a detector placed at a millimeter $r_c \sim 10^{-3} \text{m}$, this means one order of magnitude is lost for the cross section in $\Delta E_c \sim 10^{-27} \text{eV}$, evanescent indeed. Conversely, detecting this quantum tunneling with a detector sensitive to micro-electron-volts $\Delta E_c \sim 10^{-6} \text{eV} \sim 1 \mu\text{eV}$ (200 times more sensitive than the thermal energy of the cosmic microwave background) would see the cross section drop of one order of magnitude for a move of less than $10^{-13} \text{m}$, or a tenth of a pico-meter. We are at sub-atomic level of quantum tunneling: the outgoing wave evanesces into oblivion way 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 10. Analytic Continuation Annuls Sub-threshold Cross Sections.**

For massive particles, analytic continuation of above-threshold cross-section expressions to complex wavenumbers $k_c \in \mathbb{C}$ will automatically close sub-threshold channels.

**Proof.** The proof is based on the fact that massive particles are subject to mappings (2), or (4) for relativistic correction, which entail the wavenumbers are real above threshold, and exactly imaginary sub-threshold: $\forall E < E_{T_c}, k_c \in \mathbb{R}$. 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 non-relativistic Schrödinger equation applies, so that writing the conservation of probability on a control volume, and applying the Green-Ostrogradky theorem, will yield the following expression for the probability current vector:

$$\vec{j}_{\psi} := \frac{\hbar}{\mu} \Im \left[ \psi^* \nabla \psi \right] \quad \text{(129)}$$

where $\mu$ is the reduced mass of the two-particle system (c.f. equations (2.10) and (2.12) section VIII.2.A, p.312 in [4]). By definition, the differential cross section $d\sigma/d\Omega$ 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, $\psi_c(r_c) \sim e^{ik_c \cdot \vec{r}_c}$; and the outgoing channel $c'$, classically modeled as radial wave, $\psi_{c'}(r_{c'}) \sim \frac{e^{ik_{c'} \cdot \vec{r}'}}{r_{c'}}$. For arbitrary complex wavenumbers, $k_c, k_{c'} \in \mathbb{C}$, definition (129) will yield the following probability currents respectively:

$$\vec{j}_{\psi_c} \propto \frac{\hbar}{\mu} \Im \left[ k_c \right] \quad \vec{j}_{\psi_{c'}} \propto \frac{\hbar}{\mu} \Im \left[ k_{c'} \right]$$

One will note these expressions are not the imaginary part of an analytic function in the wavenumber, because of the imaginary part $\Im[k_c]$. If however we look at real wavenumbers $k_c, k_{c'} \in \mathbb{R}$, that is at above-threshold energies $E \geq E_{T_c}$, the probability currents (130) readily simplify to:

$$\vec{j}_{\psi_c} \propto \frac{\hbar}{\mu} \Re \left[ k_c \right] \quad \vec{j}_{\psi_{c'}} \propto \frac{\hbar}{\mu} \Re \left[ k_{c'} \right]$$

These expressions are the real part of analytic functions of the wavenumbers. If we analytically continue them to complex wavenumbers, and consider the cases of sub-threshold reactions $E < E_{T_c}$, for either the incoming or the outgoing channel, the wavenumbers are then exactly imaginary, $k_c, k_{c'} \in \mathbb{R}$. The real parts in (131) become zero, thereby annulling the cross section $\sigma_{c,c'}(E)$. This means that for massive particles subject to real potentials, analytic continuation of the probability currents expressions above threshold (131) will automatically close the sub-threshold channels. This is true regardless of whether the transmission matrix (117) is evanescent or not below threshold. This constitutes another major argument in favor of analytic continuation of open-channels expressions to describe the closed channels.

Note that our proof does not stand for photon channels. For photon channels, the derivations for the probability current vector (129) do not stand, and the wavenumber $k_c$ is not imaginary below threshold using mapping (3), nor using the relativistic-correction (4). The fundamental reason why photon treatment is not straightforward is that R-matrix theory was constructed on the semi-classical 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 the photons, though some works have been done to describe photons through wave functions [76, 77]. This is another open area in the field of R-matrix theory, beyond the scope of this article.
VI. CONCLUSION

In this article, we conduct a study and establish novel properties of three alternative parametrizations of the scattering matrix in R-matrix theory: the Wigner-Eisenbud parameters, the Brune parameters, and the Siegert-Humblet parameters. We link these parametrizations to the Humbert-Rosenfelt complex-pole expansion of the scattering matrix, and show that, in general, these parametrizations mark a trade-off between the complexity of the parameters and the complexity of the energy dependence of the scattering matrix.

The Wigner-Eisenbud parameters are the poles \{E_\lambda\} and residue widths \{\gamma_{\lambda,c}\} of the \(R\) matrix (17). They are \(N_\lambda \in \mathbb{N}\), simple, real poles, which are independent from one another (meaning any choice of real parameters are physically acceptable), and de-entangle the energy dependence of the \(R\) matrix from the branch-points through the multi-sheeted Riemann surface of mapping (6). Both \{E_\lambda\} and \{\gamma_{\lambda,c}\} are dependent on both the channel radii \{a_c\} and the boundary conditions \{B_c\}. The set of Wigner-Eisenbud parameters \(\{E_{T_r}, a_c, B_c, E_\lambda, \gamma_{\lambda,c}\}\) is sufficient to entirely determine the energy behavior of the scattering matrix \(U\) through (19).

The Brune parameters are the poles \(\{\bar{E}_i\}\) of the \(R_S\) matrix (37) and the widths \(\{\bar{\gamma}_{i,c}\}\), transformed by (34) from the residue widths of the physical level matrix \(\bar{A}\) in (29) and (33). They are \(N_S \geq N_\lambda\) simple, real poles, and are intimately interdependent in that not any set of real parameters is physically acceptable (they must be solutions to (33)). If definition (39) is chosen for the shift function \(S\), the Brune parameters live on the multi-sheeted Riemann surface of mapping (6): they have shadow poles \(\{\bar{E}_i\}\) on the unphysical sheets \(E, -\) below threshold \(E < E_{T_r}\), though there are only \(N_\lambda\) real poles on the physical sheet (theorem 1). If definition (41) is chosen, then the shift factor \(S\) is a function of \(\rho^2\), which unfolds the sheets in mapping (6): there are then \(N_S \geq N_\lambda\) real poles \(\{\bar{E}_i\}\), all living on the same sheet with no branch points (theorem 2). Both \(\{\bar{E}_i\}\) and \(\{\bar{\gamma}_{i,c}\}\) are invariant to change in boundary conditions \(\{B_c\}\), though both depend on the channel radii \(\{a_c\}\). Any set of \(N_\lambda\) Brune parameters \(\{E_{T_r}, a_c, \bar{E}_i, \bar{\gamma}_{i,c}\}\) is sufficient to entirely determine the energy behavior of the scattering matrix \(U\) through (32) and (19) (theorem 3).

The Siegert-Humblet parameters are the poles \(\{\tilde{E}_j\}\) and residue widths \(\{\tilde{r}_{j,c}\}\) of the Kapur-Peierls \(R_L\) operator (20). They are \(N_L \geq N_\lambda\) complex, (almost always) simple poles, that reside on the Riemann surface of mapping (6), comprised of \(2^{N_c}\) branches, and for which one must specify on which sheet they reside, as in (75). They are intimately interwoven in that not any set of complex parameters is physically acceptable (they must be solution to (55)). Both \(\{\tilde{E}_j\}\) and \(\{\tilde{r}_{j,c}\}\) are invariant to a change in channel radii \(\{a_c\}\), and we established in theorem 4 a simple way of transforming the radioactive widths \(\{\tilde{r}_{j,c}\}\) under a change of channel radius \(a_c\). Since the Siegert-Humblet parameters are the poles and residues of the local Mittag-Leffler expansion (54) of the Kapur-Peierls matrix \(R_L\), the set of Siegert-Humblet parameters \(\{E_{T_r}, a_c, \tilde{E}_j, \tilde{r}_{j,c}\}\) is insufficient to entirely determine the energy behavior of the scattering matrix \(U\) through (79) and (78). The latter expressions directly link the R-matrix parameters to the poles and residues of the Humbert-Rosenfeld expansion of the scattering matrix, and can be complemented by local coefficients \(\{s_n\}_{V(E)}\) of the entire part (80), to untangle the energy dependence of the scattering matrix into the simple sum of poles and residues (78), which is the full Humbert-Rosenfeld expansion of the scattering matrix. Theorem 7 establishes that under analytic continuation of the R-matrix operators, the poles of the Kapur-Peierls \(R_L\) operator (i.e. the Siegert-Humblet poles) are exactly the poles of the scattering matrix \(U\). The latter result constitutes one of the three arguments we here advance to argue that, contrary to the legacy force-closure of sub-threshold channels presented in Lane & Thomas [5], the scattering matrix \(U\) 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 wavefunctions, as we establish in theorem 6. Moreover, we show in theorem 8 that analytic continuation of the scattering matrix R-matrix parametrization (19) verifies Eden & Taylor’s generalized unitarity condition (107), in the wake showing that real boundary conditions \(B_c \in \mathbb{R}\) are also necessary for unitarity. Finally, we argue in theorems 9 and 10 that analytic continuation will close cross sections for massive particle channels below threshold.

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