# $K$-matrix analysis of resonance nuclear reactions

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A simple parametrization of nuclear reaction cross sections in terms of resonance parameters is obtained from the expansion of a modified $\mathcal{H}$ matrix. The latter is defined in such a way that it has no other singularity in the complex energy plane than its poles. When expanded in terms of these poles, it can be used to analyze and parametrize low-energy data on resonance reactions. The pole energies $E_\lambda$ are the resonance energies without shift (except when there is a nearby threshold of a closed neutron channel), and the residues are the products of reduced width amplitudes $g_{c\lambda}$. These two sets of parameters $(E_\lambda, g_{c\lambda})$ are independent of the channel radii and no boundary condition constants are involved in their definitions. Also, few-level approximations of the expanded $\mathcal{H}$ matrix retain the unitarity of the $S$ matrix. These properties add more reliability to the extrapolation of data to lower energies, as often necessary for reactions of astrophysical interest.

## I. INTRODUCTION

An important part of the present low-energy nuclear experiments aims at obtaining data required by open problems in nucleosynthesis.[1] In many cases, the effective stellar energy is too low to allow a direct measure of the cross section. One must then turn to theoretical approaches. One of them consists in parametrizing higher-energy data in order to obtain by extrapolation the cross section at astrophysical energies.

Several parametrizations are now available for that purpose. The simplest consists in expanding the collision matrix $S$ in terms of its poles in the complex energy plane.[2] This is certainly a very appropriate way to introduce the resonance energies and the corresponding total, reduced, and partial widths into the parametrization. But, in practice, since only few-level approximations are used, the corresponding approximate $S$ matrix has lost its unitarity property. This could make the extrapolation unreliable at low energies.

On the contrary, the few-level approximation of an $R$-matrix parametrization retains the unitarity property of the $S$ matrix.[3,4] But, on the other hand, this type of approximation introduces a dependence of $S$ on the channel radii. Moreover, the advantage of parametrizing the real $R$ matrix in terms of real parameters is made at the price of introducing energy eigenvalues which are not exactly the observed resonance energies. Like the reduced widths, they strongly depend on the boundary condition constants and on the channel radii. Useful and sensible prescriptions[5] have minimized these drawbacks, but they are not simple and most applications have been concerned with the one-channel case only.

The aim of the present paper is to introduce an alternative and simpler parametrization retaining, to the extent this is possible, the best of the above $S$ and $R$ parametrizations. We show that, if the conventional $K$ matrix is modified in an appropriate way, mainly at negative-channel energies, the resulting modified $\mathcal{H}$ matrix has only pole singularities in the complex energy plane. Accordingly, its poles and their residues, i.e., the resonance energies and the reduced widths, are independent of the channel radii. Being real and symmetrical, its few-level approximation retains the unitarity of the $S$ matrix. No boundary condition constants are introduced. The very definition of $\mathcal{H}$ eliminates *de facto* the closed channels, except the neutron ones.

A very brief account of this parametrization has been given in two earlier papers,[6,7] when it was used to parametrize the data on $^{12}C(\alpha,\gamma)^{16}O$ and $^{12}C(\alpha,\alpha)^{12}C$, in order to obtain the astrophysical $S$ factor at 0.3 MeV, i.e., well below the lowest energy at which data have been obtained ($\sim 1$ MeV).

Our general hypotheses are the conventional ones, as they are explained in the review paper by Lane and Thomas.[4] In short, we assume (1) the hermiticity of the potential energy in the Hamiltonian, so that there exists a unitary and symmetrical collision matrix, (2) the compound nucleus does not decay into more than two fragments, and (3) the configuration space of all the nucleons can be divided into an "internal" region and a channel region. This is briefly explained in the next section where our notation and definitions closely follow those of Ref. 4.

In Sec. II, we also introduce the collision matrix $S$ and the conventional $K$ matrix, the latter as a generalized collision matrix.[8] In Sec. III, we analyze the singularities of the energy dependence of the $S$ and $K$ matrices, so that in Sec. IV we can successively define a pair of linearly independent radial Coulomb wave functions $\bar{F}_l, \bar{G}_l$, which are entire functions of the energy $E$, and hence another generalized collision matrix, $\mathcal{H}$. This so-called "modified $\mathcal{H}$ matrix" is a meromorphic function of $E$. In the same section, we also give its relation to the $S$ matrix, while its expansion in terms of its poles is justified in Sec. V. In Sec. VI, we obtain the $S$ matrix corresponding to a one-level approximation of $\mathcal{H}$ and introduce the associated partial and total widths. We observe that only the closed neutron channels can introduce an energy shift in the corresponding approximate $S$ matrix of the Breit-Wigner type. In Secs. VII and VIII, we discuss the closed-

 

channel and bound-state problems, respectively. Simple results of practical importance are obtained. In Sec. IX, we observe that not all the poles are always associated with a resonance. The so-called echo poles, when there are any, contribute to the background part of $\mathcal{K}$; they are easily recognized in the elastic channel at energies where the phase shift is decreasing. Finally, Sec. X contains some concluding remarks related to the practical fitting of the parametrized $\mathcal{K}$ matrix to experimental data.

## II. THE $S$ AND $K$ MATRICES

Let $\Psi$ be the wave function of all the nucleons involved in a nuclear reaction. We assume that their center of mass is at rest and that their fragmentation into more than two nuclei can be disregarded. We can then also assume that the configuration space of all the nucleons can be divided into two parts: an "internal" region corresponding to all the nucleons being close to one another, and an "external" region, or channel region. The latter corresponds to the nucleons being divided into two nuclei, with the distance $r_c$ of their center of mass being large enough ($r_c > a_c$) so that they interact only because of the Coulomb and centrifugal forces; $a_c$ is the so-called channel radius for channel $c$. Let $\Psi_{\text{int}}, \Psi_{\text{ext}}$ designate the wave function $\Psi$ in the internal and external regions, respectively.

In channel $c$, the total energy $E$ can be decomposed as

$$E = E_c + E_\alpha \ , \tag{2.1}$$

where, in terms of the reduced mass

$$M_c = M_{\alpha_1} M_{\alpha_2} / (M_{\alpha_1} + M_{\alpha_2}) \ , \tag{2.2}$$

$E_c = \hbar^2 k_c^2 / 2M_c$ is the kinetic energy of the two nuclei in the center of mass system, while $E_\alpha = E_{\alpha_1} + E_{\alpha_2}$ is the sum of their internal energies.

Under such conditions, the surface $\mathcal{S}$ separating the internal and external regions of the configuration space is composed of partial surfaces $\mathcal{S}_c$, with $r_c = a_c$, and corresponding to the various fragmentations of the nucleons into two nuclei. Let $\Psi_{\alpha_i I_i i_i}$ $(i = 1,2)$ be the internal wave function of one nucleus, with $\alpha_i$ specifying the fragmentation and the energy state of that nucleus, and $I_i, i_i$ its spin state. We first define a channel spin-wave function as

$$\varphi_{\alpha s \nu} = \sum_{i_1 + i_2 = \nu} (I_1 I_2 i_1 i_2 | s \nu) \Psi_{\alpha_1 I_1 i_1} \Psi_{\alpha_2 I_2 i_2} \tag{2.3}$$

with $\mathbf{I}_1 + \mathbf{I}_2 = \mathbf{s}$, $|I_1 - I_2| \le s \le I_1 + I_2$, and $\alpha$ standing for $\alpha_1, \alpha_2$. The wave function of the relative motion can be given the form

$$i^l Y_{lm}(\hat{r}_c) u_c(r_c, k_c) / r_c \ . \tag{2.4}$$

The radial function $u_c$ satisfies the Coulomb equation

$$[d^2/dr_c^2 - l(l+1) r_c^{-2} + k_c^2 - U_c] u_c = 0 \ , \tag{2.5}$$

where $U_c = Z_{\alpha_1} Z_{\alpha_2} e^2 2M_c \hbar^{-2} r_c^{-1}$.

It is convenient to define, as in Ref. 4, a so-called surface function as

$$\varphi_{\alpha s l \nu m} = \varphi_{\alpha s \nu} i^l Y_{lm}(\hat{r}_c) / r_c \tag{2.6}$$

in the channel spin representation $(\alpha s l \nu m)$, and

$$\varphi_{\alpha s l J M} = \sum_{\nu + m = M} (s l \nu m | J M) \varphi_{\alpha s l \nu m} \tag{2.7}$$

in the total spin representation $(\alpha s l J M)$.

The notation $c, d, \ldots$ is used for any of the two complete sets $(\alpha s l \nu m)$ and $(\alpha s l J M)$, or for part of these quantities when no confusion can arise, e.g., $u_c$ stands for $u_{\alpha l}$, $r_c$ for $r_\alpha$.

Having excluded fragmentations into more than two nuclei, there is no overlap of the two-nuclei channels and we can assume the surface factors $\varphi_c$ to be a complete orthonormal set on the boundary surface $\mathcal{S}$. We then have

$$\int \varphi_c^* \varphi_d \, d\mathcal{S} = \int \varphi_c^* \varphi_d \, d\mathcal{S}_c = \delta_{cd} \ , \tag{2.8}$$

where

$$d\mathcal{S} = \sum_e d\mathcal{S}_e = \sum_e a_e^2 dq_{e1} dq_{e2} d\Omega_e$$

implies that, on each channel surface $r_e = a_e$, the integration is performed over the internal coordinates of both fragments and only over the angles of their relative motion.

Accordingly, in the external region, the general wave function for a two-fragment nuclear reaction has the form

$$\Psi_{\text{ext}} = \sum_c (x_c \mathcal{O}_c + y_c \mathcal{I}_c) \ , \tag{2.9}$$

where $\mathcal{O}_c, \mathcal{I}_c$ are the outgoing and incoming wave functions in channel $c$. Normalized to unit flux through a sphere of large radius $r_c$, they are

$$\begin{aligned} \mathcal{O}_c &= \varphi_c O_c(r_c, k_c) v_c^{-1/2} \ , \\ \mathcal{I}_c &= \varphi_c I_c(r_c, k_c) v_c^{-1/2} \ , \end{aligned} \tag{2.10}$$

where the $r_c^{-1}$ factor is contained in $\varphi_c$, $v_c = \hbar k_c / M_c$ is the relative velocity, while $O_c, I_c$ are the particular solutions of Eq. (2.5) corresponding to an outgoing and incoming wave, respectively.

Let us define the radial factors $V_c, D_c$ (for value and derivative) related to the value of $\Psi_{\text{int}}$ on and near the surface $\mathcal{S}_c$, namely

$$V_c = [\hbar / (2M_c)^{1/2}] \int \varphi_c^* \Psi_{\text{int}} \, d\mathcal{S} \ , \tag{2.11a}$$

$$D_c = [\hbar / (2M_c a_c^2)^{1/2}] \int \varphi_c^* \, \text{grad}_n (r_c \Psi_{\text{int}}) \, d\mathcal{S} \ , \tag{2.11b}$$

where $\text{grad}_n$ stands for the normal derivative to $\mathcal{S}$. Both $V_c$ and $D_c$ depend on the energy $E$. Since they must match the radial factors of

$$\Psi_{\text{ext}} = \sum_c \varphi_c u_c(r_c, k_c) \tag{2.12}$$

on $\mathcal{S}_c$, i.e., on the surface $r_c = a_c$, we have

$$V_c=[\hbar/(2M_c)^{1/2}]u_c(a_c,k_c)\ , \tag{2.13a}$$

$$D_c=[\hbar/(2M_c)^{1/2}](du_c/dr_c)_{r_c=a_c}\ , \tag{2.13b}$$

or,[9] according to Eqs. (2.9) and (2.10),

$$V_c=(\hbar/2k_c)^{1/2}[x_cO_c(a_c,k_c)+y_cI_c(a_c,k_c)]\ , \tag{2.14a}$$

$$D_c=(\hbar/2k_c)^{1/2}[x_c(dO_c/dr_c)_{r_c=a_c}+y_c(dI_c/dr_c)_{r_c=a_c}]\ . \tag{2.14b}$$

The normalization adopted for $O_l,I_l$ is given by their relations to the conventional Coulomb radial functions, $F_l,G_l$, namely,

$$O_l=G_l+iF_l,\quad I_l=G_l-iF_l\ . \tag{2.15}$$

With $A'=dA/dr$, these functions satisfy the Wronskian relations

$$W(G_l,F_l)\equiv G_lF_l'-G_l'F_l=k\ , \tag{2.16}$$

$$W(I_l,O_l)=2ik\ . \tag{2.17}$$

Introducing the notation

$$W(V_c,I_c;a_c)=V_c(I_c')_{r_c=a_c}-D_c(I_c)_{r_c=a_c}\ , \tag{2.18a}$$

$$W(V_c,O_c;a_c)=V_c(O_c')_{r_c=a_c}-D_c(O_c)_{r_c=a_c}\ , \tag{2.18b}$$

solving Eqs. (2.14) for $x_c,y_c$ gives

$$x_c=i(2\hbar k_c)^{-1/2}W(V_c,I_c;a_c)\ , \tag{2.19a}$$

$$y_c=-i(2\hbar k_c)^{-1/2}W(V_c,O_c;a_c)\ . \tag{2.19b}$$

Let us now consider a particular wave function $\Psi^{(c)}$ having an incoming part in channel $c$ only. If this incoming part is normalized to unit flux, $\Psi^{(c)}_{\rm ext}$ has the form

$$\Psi^{(c)}_{\rm ext}=\sum_d(\mathcal{J}_d\delta_{dc}-\mathcal{O}_dS_{dc}) \tag{2.20}$$

with, according to Eqs. (2.9) and (2.19),

$$S_{dc}=-\frac{x_d^{(c)}}{y_c^{(c)}}=\frac{W(V_d^{(c)},I_d;a_d)k_d^{-1/2}}{W(V_c^{(c)},O_c;a_c)k_c^{-1/2}}\ . \tag{2.21}$$

This ratio $S_{dc}$ is an element of the collision matrix $S$. According to Eq. (2.19b), the radial factors $V_e^{(c)},D_e^{(c)}$ of $\Psi^{(c)}$ satisfy the boundary conditions

$$W(V_e^{(c)},O_e;a_e)=0\quad(\text{all } e\neq c)\ . \tag{2.22}$$

Equations (2.9)–(2.14) and (2.20)–(2.22) can also be applied when $I_l,O_l$ are defined as linear combinations of $F_l,G_l$ different from Eqs. (2.15), provided

$$W(I_l^{\rm new},O_l^{\rm new})/k \tag{2.23}$$

has the same value in all channels. The ratio corresponding to the right-hand side (rhs) of Eq. (2.21) is then an element of a generalized collision matrix.[8] In particular, when $I_l^{\rm new},O_l^{\rm new}$ are chosen to be the real functions $F_l,-G_l$, the ratio (2.21) becomes

$$K_{dc}=-\frac{W({}^KV_d^{(c)},F_d;a_d)k_d^{-1/2}}{W({}^KV_c^{(c)},G_c;a_c)k_c^{-1/2}} \tag{2.24}$$

with the radial factors ${}^KV_e^{(c)},{}^KD_e^{(c)}$ satisfying the real boundary conditions

$$W({}^KV_e^{(c)},G_e;a_e)=0\quad(\text{all } e\neq c)\ . \tag{2.25}$$

$K_{dc}$ is an element of the conventional $K$ matrix related to $S$ by the equation

$$S=(1+iK)(1-iK)^{-1}\ . \tag{2.26}$$

## III. THE SINGULARITIES OF $S$ AND $K$ MATRICES

The $S$ and $K$ matrices are unambiguously defined when the channel energy $\hbar^2k_c^2/2M_c$ is positive in all channels. But, negative and even complex energies must also be considered, and the radial Coulomb wave functions $F_l$, $G_l$, $I_l$, $O_l$ have singularities at $k=0$ and for imaginary values of $k$, i.e., for $k^2<0$. Let us display these singularities and see how they can best be accounted for.

Introducing the Sommerfeld parameter

$$\eta=\alpha/k,\quad \alpha=Z_1Z_2e^2M\hbar^{-2}>0 \tag{3.1}$$

and the conventional notation

$$\rho=kr,\quad x=(8\eta\rho)^{1/2}=(8\alpha r)^{1/2}\ , \tag{3.2}$$

let us define the auxiliary functions of $\eta$:

$$C_0(\eta)=[2\pi\eta/(e^{2\pi\eta}-1)]^{1/2}\ , \tag{3.3a}$$

$$u_l(\eta)=(1+\eta^{-2})(1+4\eta^{-2})\cdots(1+l^2\eta^{-2})\ ,\quad u_0=1\ , \tag{3.3b}$$

$$\varepsilon_l(\eta)=\eta^lC_0(\eta)u_l(\eta)^{1/2}/l!,\quad \varepsilon_l(0)=1\ , \tag{3.3c}$$

$$h(\eta)=\tfrac{1}{2}\psi(1+i\eta)+\tfrac{1}{2}\psi(1-i\eta)-\ln\eta\ , \tag{3.3d}$$

$$f(\eta)=2\eta C_0^{-2}(\eta)h(\eta)=\frac{1}{\pi}(e^{2\pi\eta}-1)h(\eta)\ , \tag{3.3e}$$

where $\psi$ is the digamma function.[10] With these definitions, $F_l,G_l$ can be given the form[11]

$$F_l=(\varepsilon_lk^{l+1})\tfrac{1}{2}l!\alpha^{-l-1}(x/2)^{2l+2}\Phi_l(x,\eta^{-2})\ , \tag{3.4a}$$

$$G_l=(\varepsilon_lk^l)^{-1}(l!)^{-1}\alpha^l(x/2)^{2l+2}\times[h(\eta)u_l(\eta)\Phi_l(x,\eta^{-2})+\Omega_l(x,\eta^{-2})] \tag{3.4b}$$

$$=fF_l+(\varepsilon_lk^l)^{-1}(l!)^{-1}\alpha^l(x/2)^{2l+2}\Omega_l(x,\eta^{-2})\ . \tag{3.5}$$

On the one hand, $\Phi_l,\Omega_l$ are entire[12] functions in $\eta^{-2}$, i.e., they have no singularity at real or complex values of $k^2$ if $|k^2|<\infty$. But, on the other hand, it is obvious that $F_l,G_l$ have an infinite number of singularities for finite values of $k$: singular branchpoints in $C_0u_l^{1/2}$ and poles in $\psi(1\pm i\eta)$, while $k=0$ is an essential and logarithmic singularity.

Under such conditions, the $K$-matrix element (2.24) has no simple pole expansion that could be used to parametrize cross sections. One can isolate the singular threshold factors $F_l,G_l$ [the first factors in Eqs. (3.4)] and consider expanding the ratio $K_{dc}/\varepsilon_ck_c^{l_c+1}\varepsilon_dk_d^{l_d}$, rather than $K_{dc}$ itself, as it has been done for $S_{dc}$ in Ref. 13. But, that does not remove the singularities of $h(\eta)$ in $\varepsilon_lk^lG_l$, so that cuts must be introduced in the complex $E$ plane. However, a much simpler parametrization can be

achieved if the singularities of $h(\eta)$ are eliminated by substituting an *ad hoc* linear combination of $F_l$ and $G_l$ for $G_l$. This is possible because of the very form of the rhs of Eq. (3.5), $h(\eta)$ being in the $f$ factor only.

Two linear combinations of $F_l, G_l$ which are entire functions of $k^2$ (i.e., without singularity for $|k^2|<\infty$) are

$$\bar{F}_l = F_l/\varepsilon_l k^{l+1} = \tfrac{1}{2} l! \alpha^{-l-1}(x/2)^{2l+2}\Phi_l(x,\eta^{-2}) , \quad (3.6a)$$

$$\bar{G}_l = (l!)^{-1}\alpha^l (x/2)^{2l+2}[h_N(\eta)u_l(\eta)\Phi_l(x,\eta^{-2}) + \Omega_l(x,\eta^{-2})] \quad (3.6b)$$

$$= \varepsilon_l k^l G_l - 2(l!)^{-2}\alpha^{2l+1}u_l(\eta)[h(\eta)-h_N(\eta)]\bar{F}_l \quad (3.7a)$$

$$= \varepsilon_l k^l [G_l - (f-f_N)F_l] , \quad (3.8)$$

where $h_N(\eta)$ is a polynomial of degree $N$ in $\eta^{-2}$ whose precise definition is given in the Appendix, while

$$f_N(\eta) = 2\eta C_0^{-2}(\eta) h_N(\eta) . \quad (3.9)$$

In short, the functions $\bar{F}_l, \bar{G}_l$ differ from $F_l, G_l$ by the fact that they have been divided by their respective $\eta$-dependent threshold factors and also by the polynomial $h_N(\eta)$ having been substituted for the singular function $h(\eta)$ in $G_l$.

Defining also

$$h^+(\eta) = h(\eta) + i\pi/(e^{2\pi\eta}-1) , \quad (3.10)$$

it is useful to rewrite Eq. (3.7a) in the form

$$\bar{G}_l = \varepsilon_l k^l (G_l + iF_l) - 2(l!)^{-2}\alpha^{2l+1}u_l(\eta)[h^+(\eta)-h_N(\eta)]\bar{F}_l . \quad (3.7b)$$

The very definition of the polynomial $h_N(\eta)$ is such that *at finite positive energies* $|h(\eta)-h_N(\eta)|$ is arbitrarily small, so that $h(\eta)-h_N(\eta)$ is numerically negligible. *At finite negative energies* $[k=ib\ (b\geq 0),\ i\eta=\beta>0]$

$$h^+(\eta) = \psi(\beta) + \frac{1}{2\beta} - \ln\beta ,$$

and it is $|h^+(\eta)-h_N(\eta)|$ that is arbitrarily small. So, numerically in practice in Eq. (3.7a), we have

$$h(\eta)-h_N(\eta)=0 \quad (k^2>0) \quad (3.11a)$$

at positive energies, and in Eq. (3.7b),

$$h^+(\eta)-h_N(\eta)=0 \quad (k^2<0) \quad (3.11b)$$

at negative energies; in both Eqs. (3.7), $u_l(\eta), \bar{F}_l$ remain bounded at finite energies.

From Eqs. (2.16), (3.6a), and (3.8), the Wronskian relation satisfied by $\bar{F}_l, \bar{G}_l$ is

$$W(\bar{G}_l, \bar{F}_l) = 1 . \quad (3.12)$$

Up to now, in this section, we have assumed $\alpha>0$. When $\alpha=0$, i.e., in a neutron channel, we have $\eta=0$ and hence[14]

$$F_l = (\tfrac{1}{2}\pi kr)^{1/2} J_{l+1/2}(kr) , \quad (3.13a)$$

$$G_l = (-)^l (\tfrac{1}{2}\pi kr)^{1/2} J_{-l-1/2}(kr) . \quad (3.13b)$$

Dividing these functions by their threshold factors, $k^{l+1}$ and $k^{-l}$, respectively, we obtain

$$\bar{F}_l = (\tfrac{1}{2}\pi r)^{1/2} k^{-l-1/2} J_{l+1/2}(kr) , \quad (3.14a)$$

$$\bar{G}_l = (-)^l (\tfrac{1}{2}\pi r)^{1/2} k^{l+1/2} J_{-l-1/2}(kr) . \quad (3.14b)$$

Both are entire functions of $k^2$, as is easily seen from their respective power expansions. They also satisfy Eq. (3.12).

## IV. THE MODIFIED $\mathcal{K}$ MATRIX

The generalized collision matrix $\mathcal{K}$ corresponds to the choice of $\bar{F}_l, -\bar{G}_l$ as a pair of linearly independent Coulomb functions in the channel region. The value of the Wronskian of this pair being, like that of the pair $I_l k^{-1/2}, O_l k^{-1/2}$, the same in all channels, the matrix elements of $\mathcal{K}$ are obtained when the substitutions

$$I_l k^{-1/2}, O_l k^{-1/2} \Longrightarrow \bar{F}_l, -\bar{G}_l \quad (4.1)$$

are made in Eqs. (2.14). This gives

$${}^{\mathcal{K}}x_c = -(2/\hbar)^{1/2} W({}^{\mathcal{K}}V_c, \bar{F}_c; a_c) . \quad (4.2a)$$

$${}^{\mathcal{K}}y_c = -(2/\hbar)^{1/2} W({}^{\mathcal{K}}V_c, \bar{G}_c; a_c) . \quad (4.2b)$$

Let ${}^{\mathcal{K}}V_e^{(c)}, {}^{\mathcal{K}}D_e^{(c)}$ be the radial factors corresponding to the wave function having an "incoming" part (in $\bar{F}_c$) only in channel $c$. They are functions of $E$ and satisfy the conditions

$$W({}^{\mathcal{K}}V_e^{(c)}, \bar{G}_e; a_e) = 0 \quad (\text{all } e \neq c) \quad (4.3)$$

which correspond to Eqs. (2.22). From Eqs. (4.2), the amplitude ratio $-{}^{\mathcal{K}}x_d^{(c)}/{}^{\mathcal{K}}y_d^{(c)}$ is

$$\mathcal{K}_{dc} = -\frac{W({}^{\mathcal{K}}V_d^{(c)}, \bar{F}_d; a_d)}{W({}^{\mathcal{K}}V_c^{(c)}, \bar{G}_c; a_c)} \quad (4.4)$$

as also results from the direct substitution (4.1) being made into Eq. (2.21). This is an element of the $\mathcal{K}$ matrix. It gives the amplitude of an "outgoing" wave (in $\bar{G}_d$) in channel $d$ generated by an "incoming" wave (in $\bar{F}_c$) of unit amplitude in channel $c$. From Eq. (4.3), we also have

$$\mathcal{K}_{dc} = -\delta_{dc}\bar{F}_c/\bar{G}_c - \frac{{}^{\mathcal{K}}V_d^{(c)}/\bar{G}_d}{W({}^{\mathcal{K}}V_c^{(c)}, \bar{G}_c; a_c)} . \quad (4.5)$$

In order to obtain the relation between the $S$ and $\mathcal{K}$ matrices, we must find the coefficients in the linear relations

$$\bar{F}_l = \xi_l I_l k^{-1/2} + \lambda_l O_l k^{-1/2} , \qquad \bar{G}_l = \zeta_l I_l k^{-1/2} + \chi_l O_l k^{-1/2} . \quad (4.6)$$

Defining, when $\alpha>0$,

$$p_l = \varepsilon_l(\eta) k^{l+1/2} , \quad (4.7)$$

they are given by

$$\xi_l=-\lambda_l=\tfrac{1}{2}ip_l^{-1}\ , \tag{4.8a}$$

$$\zeta_l=-\tfrac{1}{2}p_l[1-i(f-f_N)]\ ,$$
$$\chi_l=-\tfrac{1}{2}p_l[1+i(f-f_N)]\ . \tag{4.8b}$$

We also define

$$\mu_l=-i\xi_l^{-1}\zeta_l=p_l^2[1-i(f-f_N)]\ . \tag{4.9}$$

Because $\varepsilon_l(\eta)\to 1$, $f(\eta)\to 0$ for $\eta\to 0$, the formulas (4.6)–(4.9) remain valid for a neutron channel provided 0 is substituted for $f_N(\eta)$ in Eqs. (4.8b) and (4.9). In this case, we have

$$p_l=k^{l+1/2},\quad \mu_l=k^{2l+1}\ . \tag{4.10}$$

Let us also introduce a matrix notation for the functions just defined, so that $p,\xi,\lambda,\ldots$ stand for diagonal matrices with elements $p_e,\xi_e,\lambda_e,\ldots$ in channel $e$, respectively.

The relation between the $S$ matrix and the generalized collision matrix $\mathcal{K}$ is[8]

$$S=(\chi\mathcal{K}-\lambda)(\xi-\zeta\mathcal{K})^{-1}\ , \tag{4.11}$$

hence,

$$T=1-S=-2ip\mathcal{K}(1-i\mu\mathcal{K})^{-1}p \tag{4.12a}$$

$$=-2ip(1-i\mathcal{K}\mu)^{-1}\mathcal{K}p \tag{4.12b}$$

and

$$\mathcal{K}=ip^{-1}[2+(S-1)\mu p^{-2}]^{-1}(1-S)p^{-1} \tag{4.13a}$$

$$=ip^{-1}(1-S)[2+p^{-2}\mu(S-1)]^{-1}p^{-1}\ . \tag{4.13b}$$

Like the $S$ matrix, the $\mathcal{K}$ matrix is independent of the channel radii because its elements are also ratios of two amplitudes.[15,16] This is in agreement with the fact that, in the relations (4.12) and (4.13), both $p$ and $\mu$ depend on the $\eta$ only.

The radial functions $u_d(r_d,k_d)$, $\bar{F}_d$, $\bar{G}_d$ being real at any real energy, so are the radial factors ${}^{\mathcal{K}}V_d^{(c)}$, ${}^{\mathcal{K}}D_d^{(c)}$ and the $\mathcal{K}$ matrix itself. Hence, when the energy $E$ is complex, all these functions and the $\mathcal{K}$ matrix have the property

$$A^*(E)=A(E^*)\ . \tag{4.14}$$

Moreover, we assume that, as in the one-channel case,[17] the existence of finite channel radii and our definitions entail that, like $\bar{F}_l,\bar{G}_l$, the radial factors ${}^{\mathcal{K}}V_d^{(c)}$, ${}^{\mathcal{K}}D_d^{(c)}$ (any $c,d$) are entire functions of $E$. Consequently, the elements of $\mathcal{K}$ are meromorphic[12] functions of $E$, i.e., they have no other singularities than isolated poles for $|E|<\infty$.

Comparing Eqs. (4.4) and (4.5), we see that for $d\neq c$, the amplitude ${}^{\mathcal{K}}V_d^{(c)}/\bar{G}_d$ is also an entire function of $E$. Except for a factor $-(2/\hbar)^{1/2}$, this ratio, like the numerator in Eq. (4.4), is the *amplitude* of the "outgoing" wave in channel $d$, in which there is no "incoming" part in $\bar{F}_d$.

## V. THE POLE EXPANSION OF $\mathcal{K}$

From Eq. (4.4), we see that the poles $E_\lambda$ of $\mathcal{K}_{dc}$ satisfy the equation

$$W({}^{\mathcal{K}}V_c^{(c)},\bar{G}_c;a_c)=0\ . \tag{5.1}$$

Together with the conditions (4.3), this amounts to say that the poles are the energies at which the general wave function $\Psi$ satisfies *all* the boundary conditions

$$W({}^{\mathcal{K}}V_e,\bar{G}_e;a_e)=0\quad(\text{all } e)\ . \tag{5.2}$$

Accordingly, the pole $E_\lambda$ of $\mathcal{K}_{dc}$ and the corresponding wave function $\Psi^{(c)}(E_\lambda)$ are independent of the entrance channel $c$. Hence, we can use the notation $\Psi_\lambda$ for $\Psi^{(c)}(E_\lambda)$, and $\Psi_\lambda$ has no "incoming" part in any channel.

From now on, we use the notation

$$A_\lambda=(A)_{E=E_\lambda} \tag{5.3}$$

so that ${}^{\mathcal{K}}V_{e\lambda}$, ${}^{\mathcal{K}}D_{e\lambda}$ designate ${}^{\mathcal{K}}V_e^{(c)}(E_\lambda)$, ${}^{\mathcal{K}}D_e^{(c)}(E_\lambda)$, respectively.

The $E_\lambda$ are assumed to be simple poles, real or complex. When $E_\lambda$ is complex, $E_\lambda^*$ is also a pole according to the property (4.14). Let us designate the corresponding wave function by $\Psi_{-\lambda}=\Psi(E_\lambda^*)$.

Under such conditions, and by analogy with the one-channel case,[17] we can expand the matrix element $\mathcal{K}_{dc}$ in terms of its poles in the form[18]

$$\mathcal{K}_{dc}=\sum_{\lambda=1}^{\infty}R_{dc\lambda}\Big/(E_\lambda-E)\ , \tag{5.4}$$

where $R_{dc\lambda}$ are constants which, as we now show, can be factorized in terms of the channel amplitudes.

As in other parametrizations,[4,13] this is obtained from Green's theorem. With $E_1,E_2$ being two different total energies $E$ and $\Psi_1=\Psi(E_1)$, $\Psi_2=\Psi(E_2)$, it reads

$$(E_2^*-E_1)\int_\omega\Psi_2^*\Psi_1 d\omega=\sum_e[V_e^*(E_2)D_e(E_1)-D_e^*(E_2)V_e(E_1)]\ , \tag{5.5}$$

where the integration extends over the internal region of the configuration space. Here, we apply it with $\Psi_1=\Psi^{(c)}(E)$ and $\Psi_2=\Psi^{(c)}(E_\lambda^*)=\Psi_{-\lambda}$ (if $E_\lambda$ is real, we simply have $\Psi_2=\Psi_{-\lambda}\equiv\Psi_\lambda$). Using Eq. (4.14), Eq. (5.5) becomes

$$(E_\lambda-E)\int_\omega\Psi_{-\lambda}^*\Psi^{(c)}d\omega=\sum_e[{}^{\mathcal{K}}V_{e\lambda}{}^{\mathcal{K}}D_e^{(c)}(E)-{}^{\mathcal{K}}D_{e\lambda}{}^{\mathcal{K}}V_e^{(c)}(E)]\ . \tag{5.6}$$

Introducing the notation

$$L_e=\bar{G}_e'(a_e,k_e)/\bar{G}_e(a_e,k_e),\quad L_{e\lambda}=(L_e)_{E=E_\lambda} \tag{5.7}$$

and taking Eq. (5.2) into account, the quantity inside the brackets in Eq. (5.6) is easily rewritten as

$$
\begin{aligned}
&{}^{\mathcal{K}}V_{e\lambda}\,{}^{\mathcal{K}}V_e^{(c)}(E)[{}^{\mathcal{K}}D_e^{(c)}(E)/{}^{\mathcal{K}}V_e^{(c)}(E)-L_{e\lambda}] \\
&\quad={}^{\mathcal{K}}V_{e\lambda}\,{}^{\mathcal{K}}V_e^{(c)}(E)(L_e-L_{e\lambda}) \\
&\qquad-\frac{{}^{\mathcal{K}}V_{e\lambda}}{\bar{G}_e(a_e,k_e)}W({}^{\mathcal{K}}V_e^{(c)}(E),\bar{G}_e;a_e)\ .
\end{aligned}
$$

Using Eq. (4.3), Eq. (5.6) now reads

$$
\begin{aligned}
&(E_\lambda-E)\int_\omega \Psi^*_{-\lambda}\Psi^{(c)}d\omega \\
&\quad=\sum_e {}^{\mathcal{K}}V_{e\lambda}\,{}^{\mathcal{K}}V_e^{(c)}(E)(L_e-L_{e\lambda}) \\
&\qquad-\frac{{}^{\mathcal{K}}V_{c\lambda}}{\bar{G}_c(a_c,k_c)}W({}^{\mathcal{K}}V_c^{(c)}(E),\bar{G}_c;a_c)\ . \qquad (5.8)
\end{aligned}
$$

Successively taking the derivative $d/dE$ of both sides of this equation, making $E=E_\lambda$, and defining

$$\dot{A}=dA/dE\ , \qquad (5.9)$$

we are left with

$$
\begin{aligned}
-\int_\omega \Psi^*_{-\lambda}\Psi_\lambda d\omega&=\sum_e {}^{\mathcal{K}}V_{e\lambda}^2\dot{L}_{e\lambda} \\
&\quad-\frac{{}^{\mathcal{K}}V_{c\lambda}}{\bar{G}_{c\lambda}}\left[\frac{d}{dE}W({}^{\mathcal{K}}V_c^{(c)}(E),\bar{G}_c;a_c)\right]_{E=E_\lambda}\ ,
\end{aligned}
$$

where $\bar{G}_{c\lambda}=\bar{G}_c(a_c,k_{c\lambda})$.

From Eq. (4.5), the residue in Eq. (5.4) is

$$
R_{dc\lambda}={}^{\mathcal{K}}V_{d\lambda}\bar{G}^{-1}_{d\lambda}\left[\frac{d}{dE}W({}^{\mathcal{K}}V_c^{(c)}(E),\bar{G}_c;a_c)\right]^{-1}_{E=E_\lambda}\ . \qquad (5.10)
$$

Defining

$$\nu_\lambda=\int_\omega \Psi^*_{-\lambda}\Psi_\lambda d\omega+\sum_e {}^{\mathcal{K}}V_{e\lambda}^2\dot{L}_{e\lambda} \qquad (5.11a)$$

$$=\int_\omega \Psi^*_{-\lambda}\Psi_\lambda d\omega+\sum_e \frac{{}^{\mathcal{K}}V_{e\lambda}^2}{\bar{G}^{\,2}_{e\lambda}}W(\bar{G}_{e\lambda},\dot{\bar{G}}_{e\lambda};a_e) \qquad (5.11b)$$

and

$$g_{c\lambda}=\frac{{}^{\mathcal{K}}V_{c\lambda}}{\bar{G}_{c\lambda}\nu_\lambda^{1/2}}\ , \qquad (5.12)$$

the expansion (5.4) now reads

$$\mathcal{K}_{dc}=\sum_{\lambda=1}^{\infty}g_{d\lambda}g_{c\lambda}/(E_\lambda-E)\ . \qquad (5.13)$$

This result proves the symmetry property of the modified $\mathcal{K}$ matrix. The independence of $\mathcal{K}$ on the channel radii entails the same property for $E_\lambda$, $g_{d\lambda}$, $g_{c\lambda}$, and $\nu_\lambda$. But, for the latter quantity, this independence can also be verified directly, as in Ref. 16, using here the relation

$$\frac{d}{dr_e}W(\bar{G}_e,\dot{\bar{G}}_e;r_e)=-\frac{2M_e}{\hbar^2}\bar{G}_e^{\,2}\ . \qquad (5.14)$$

In matrix notation, with the vector $g_\lambda$ $(g_{a\lambda},g_{b\lambda},\ldots)$ the expansion of $\mathcal{K}$ reads

$$\mathcal{K}=\sum_{\lambda=1}^{\infty}g_\lambda\times g_\lambda/(E_\lambda-E)\ . \qquad (5.15)$$

## VI. PARTIAL AND TOTAL WIDTHS, ENERGY SHIFT

In Eq. (4.12), $\mathcal{K}$, $p$, and $\mu$ are independent of the channel radii, but the very form of this matrix relation is similar to the one obtained in $R$-matrix theory, $R$ being also a generalized collision matrix. Here, from this analogy, we expect $p_l$ to play the part of a penetration factor and $i\mu_l$ that of $(aO_l'/O_l)_{r=a}$. Accordingly, let us define the real and diagonal matrices $\mathcal{S},\mathcal{P}$ by

$$i\mu=\mathcal{S}+i\mathcal{P}\ . \qquad (6.1)$$

From the definitions (4.9), (3.3), (3.9), and (3.10), we have

$$i\mu_l=ip_l^2+2(l!)^{-2}\alpha^{2l+1}u_l(\eta)(h-h_N) \qquad (6.2a)$$

$$=2(l!)^{-2}\alpha^{2l+1}u_l(\eta)(h^+-h_N)\ , \qquad (6.2b)$$

so that, from Eq. (3.11a), in an open channel $c^+$, we have, in practice,

$$\mathcal{S}_{c^+}=0,\quad \mathcal{P}_{c^+}=p_l^2\ , \qquad (6.3a)$$

while, from Eq. (3.11b), in a closed channel $c^-$

$$\mu_{c^-}=\mathcal{S}_{c^-}=\mathcal{P}_{c^-}=0 \qquad (6.3b)$$

provided $c^-$ is not a closed neutron channel.

In an open neutron channel, according to Eqs. (4.10), Eqs. (6.3a) still hold with $p_l^2=k^{2l+1}$, but in a closed neutron channel with

$$b_c=-ik_c>0,\quad \mu_c=(-)^l ib_c^{2l+1}\ , \qquad (6.4a)$$

we have

$$\mathcal{P}_{c^-}=0,\quad \mathcal{S}_{c^-}=(-)^{l+1}b_c^{2l+1}\ . \qquad (6.4b)$$

The physical consequences of these results are best seen when considering the one-level approximation of the $\mathcal{K}$ matrix, i.e., by assuming that, in the neighborhood of a real pole $E_\lambda$, a good approximation to $\mathcal{K}$ is $g_\lambda\times g_\lambda/(E_\lambda-E)$. The matrix inversion is easily performed in that case and one obtains

$$
\begin{aligned}
&\mathcal{K}(1-i\mu\mathcal{K})^{-1} \\
&\quad=g_\lambda\times g_\lambda\Big/\left[E_\lambda-\sum_e \mathcal{S}_e g_{e\lambda}^2-E-i\sum_e \mathcal{P}_e g_{e\lambda}^2\right]\ . \qquad (6.5)
\end{aligned}
$$

Let us introduce partial and total widths defined as

$$\Gamma_{e\lambda}=2p_e^2g_{e\lambda}^2,\quad \Gamma_\lambda=\sum_{e^+}\Gamma_{e\lambda}\ , \qquad (6.6)$$

where, according to Eq (6.3b), the sum extends over open channels only, and the level-shift function $\Delta_\lambda$ as

$$\Delta_\lambda=\sum_{e_N^-}(-)^{l_e}b_e^{2l_e+1}g_{e\lambda}^2 \qquad (6.7)$$

with the sum extending over closed neutron channels

only, according to Eqs. (6.3b) and (6.4b). For an element of the $T$ matrix, we have

$$T_{dc}=i\frac{\Gamma_{d\lambda}^{1/2}\Gamma_{c\lambda}^{1/2}}{E-(E_\lambda+\Delta_\lambda)+\frac{1}{2}i\Gamma_\lambda} . \tag{6.8}$$

The shift $\Delta_\lambda$ is negligible when closed neutron channel thresholds are not too close above $E_\lambda$. This results from the fact that, in $g_{e\lambda}$ defined by Eq. (5.12), the factor $\bar{G}_{e\lambda}^{-1}$ becomes negligible when

$$-ik_{e\lambda}a_e=b_{e\lambda}a_e\gg 1 .$$

From Eq. (3.14b), we have[19]

$$\bar{G}_{e\lambda}=(-)^{l_e}(\tfrac{1}{2}\pi a_e)^{1/2}b_{e\lambda}^{l_e+1/2}I_{-l_e-1/2}(b_{e\lambda}a_e) \tag{6.9a}$$

$$=(-)^{l_e}\tfrac{1}{2}b_{e\lambda}^{l_e}\exp(b_{e\lambda}a_e)[1+O(1/b_{e\lambda}a_e)] . \tag{6.9b}$$

On the other hand, in $g_{e\lambda}$, both the numerator and the denominator of ${}^{\mathcal{R}}V_{e\lambda}/\nu_\lambda^{1/2}$ depend primarily on the interior wave function $\Psi_{\text{int}}$, and this *ratio* has no exponential energy dependence. In the one-channel case, for a square well potential with depth $\mathcal{V}_0$ and range $a$, we have verified it analytically.[20] We obtained

$$g_{l\lambda}^2=8a[\mathcal{V}_0-(b_{l\lambda}\hbar^2/2Ma)^2\mathcal{V}_0^{-1}]$$
$$\times b_{l\lambda}^{-2l}\exp(-2b_{l\lambda}a)\times[1+O(1/b_{l\lambda}a)] . \tag{6.10}$$

So, more often than not, in a Breit-Wigner cross section deduced from a modified $\mathcal{R}$ matrix, there is no energy shift and no distinction is to be made between formal and observed widths.

When $E_\lambda$ is complex, the terms in $E_\lambda$ and $E_\lambda^*$ must obviously be associated with a single resonance characterized by twice the number of parameters (their real and imaginary parts) introduced by a real pole. In practice, it is very unlikely that as many parameters should ever be required to fit an observed resonance.

## VII. OPEN AND CLOSED CHANNELS

We now consider the element $T_{dc}$ of the matrix defined by Eq. (4.12a); it reads

$$T_{dc}=-2ip_d\sum_e \mathcal{R}_{de}N_{ec}p_c , \tag{7.1}$$

where $N_{ec}$ is an element of the matrix $N=D^{-1}$ with $D=1-i\mu\mathcal{R}$. The physically interesting elements of $T$ are, of course, those with $c,d$ being both open channels, but the sum over $e$ must be extended over all open and closed channels as well. As we shall now see a major simplification arises because, by an appropriate choice of $h_N(\eta)$, $\mu_e$ has been made arbitrarily small and numerically negligible in closed channels. However, since this does not apply to neutron channels, let us, in this section, divide all the channels into two groups, characterized by $+$ and $-$ signs, and having $\mu_e\neq 0$ and $\mu_e=0$, respectively. According to Eqs. (6.2)–(6.4), this implies that all the neutron channels (open or closed) are in the same group as the open channels in which the particles are both charged.

Using block matrices to represent $\mathcal{R}$, $D$, and $N$, we have

$$\mathcal{R}=\begin{bmatrix}\mathcal{R}^{++} & \mathcal{R}^{+-}\\ \mathcal{R}^{-+} & \mathcal{R}^{--}\end{bmatrix},\quad D=\begin{bmatrix}D^{++} & D^{+-}\\ 0 & 1\end{bmatrix} . \tag{7.2}$$

Considering the cofactors of $D$, we see that its inverse $N$ has the same form

$$N=\begin{bmatrix}N^{++} & N^{+-}\\ 0 & 1\end{bmatrix}, \tag{7.3}$$

hence,

$$\mathcal{R}(1-i\mu\mathcal{R})^{-1}=\begin{bmatrix}\mathcal{R}^{++}N^{++} & \mathcal{R}^{++}N^{+-}+\mathcal{R}^{+-}\\ \mathcal{R}^{-+}N^{++} & \mathcal{R}^{-+}N^{+-}+\mathcal{R}^{--}\end{bmatrix} . \tag{7.4}$$

Since $\det D=\det D^{++}$ and $N^{++}=(D^{++})^{-1}$, we have

$$[\mathcal{R}(1-i\mu\mathcal{R})^{-1}]^{++}=\mathcal{R}^{++}(1-i\mu^+\mathcal{R}^{++})^{-1} . \tag{7.5}$$

With the same channel separation also being applied to the $S$ and $T$ matrices, we now have

$$T^{++}=1-S^{++}=-2ip^+\mathcal{R}^{++}(1-i\mu^+\mathcal{R}^{++})^{-1}p^+ . \tag{7.6}$$

This result is important. It shows that the $e^-$ channels do not contribute to the sum in Eq. (7.1), or equivalently, that the closed channels of charged particles are not involved in a $\mathcal{R}$-matrix parametrization. The "closed-channel elimination" is here embedded in the very definition of the modified $\mathcal{R}$ matrix, as far as charged-particle channels are concerned. Equation (7.6) is, of course, the one to be used in the parametrization of a cross section in terms of a $\mathcal{R}$ matrix.

## VIII. BOUND STATES

Let us now see that the $\mathcal{R}$ matrix is well adapted to fitting data on a reaction when the compound nucleus has a bound state below the threshold of the entrance channel $c$. At first sight, a $\mathcal{R}$-matrix parametrization does not seem better adapted than a more conventional one, since the very form of the condition (5.1) satisfied by the $E_\lambda$ seems to be unrelated to a bound-state condition, i.e., to a vanishing denominator of $S_{dc}$ in Eq. (2.21).

Assuming that $c$ is a charged-particle channel whose threshold energy $\mathcal{E}_c$ is above the energy $E_\lambda$ of a real pole, we have

$$E_\lambda-\mathcal{E}_c=\hbar^2k_{c\lambda}^2/2M_c<0 , \tag{8.1a}$$

with

$$-ik_{c\lambda}=b_{c\lambda}>0,\quad i\eta_{c\lambda}=\beta_{c\lambda}>0 . \tag{8.1b}$$

According to Eqs. (2.15), (3.7b), and (3.11b), *at negative energies* in channel $c$, Eq. (5.1) can be given the form

$$W({}^{\mathcal{R}}V_c^{(c)},O_c;a_c)=0 , \tag{8.2}$$

which is , in fact, a bound-state condition. The radial factors ${}^{\mathcal{R}}V_c^{(c)}$, ${}^{\mathcal{R}}D_c^{(c)}$ are matched at $r_c=a_c$ with functions

in $O_c, O_c'$, respectively, with

$$O_c \propto \exp[ik_{c\lambda}r_c - i\eta_{c\lambda}\ln(2k_{c\lambda}r_c)]$$
$$\propto \exp[-b_{c\lambda}r_c - \beta_{c\lambda}\ln(2b_{c\lambda}r_c)] \quad (8.3)$$

when $b_{c\lambda}r_c \gg 1$. Consequently, if a bound state of a compound nucleus has been observed at some excitation energy $E_\lambda$, the same energy must be taken as that of a real pole in the expansion of the $\mathcal{K}$ matrix.

We also note that when a real pole $E_\lambda$ is below the threshold of a charged-particle channel $e$, $\bar{G}_{e\lambda}$ is exponentially decreasing at large $r_e$, according to Eq. (8.3). In $\nu_\lambda$ defined by Eqs. (5.11), we can then as well extend the volume integral into that channel $e$, i.e., to $r_e \to +\infty$. If this is done at all such channels, we then have

$$\nu_\lambda = \int_{\omega_\lambda} \Psi_\lambda^* \Psi_\lambda d\omega + \sum_{e^+} {}^{\mathcal{K}}V_{e\lambda}^2 \dot{L}_{e\lambda} , \quad (8.4)$$

where $\omega_\lambda$ designates the extended domain of integration, while $e^+$ designates all the other channels, i.e., the charged-particle channels for which the condition $E_\lambda - \mathcal{E}_e < 0$ is not satisfied and all the neutron channels.

Moreover, when $E_\lambda$ is below all channel thresholds, and if the neutron channel thresholds are well above $E_\lambda$ so that they can be ignored, $E_\lambda$ is a bound state of the compound nucleus and we have

$$\nu_\lambda = \int_{\omega_\lambda} \Psi_\lambda^* \Psi_\lambda d\omega > 0 . \quad (8.5)$$

Hence, we can conclude that, in this case,

$$g_{e\lambda}^2 > 0 \quad (8.6)$$

in all channels. The importance of this result will be seen in Sec. IX.

## IX. RESONANCES AND ECHO POLES

In the expansion of the diagonal element $\mathcal{K}_{cc}$, the pole terms have the form $g_{c\lambda}^2/(E_\lambda - E)$. Is $g_{c\lambda}^2$ always positive when $E_\lambda$ is real? According to Eq. (5.12), this depends on the sign of $\nu_\lambda$. This can be more easily discussed if we first turn to the elastic scattering by a central potential.

In this case, both $\mathcal{K}$ and $S$ are diagonal. We have

$$\mathcal{K}_l = -\frac{W({}^{\mathcal{K}}V_l, \bar{F}_l; a)}{W({}^{\mathcal{K}}V_l, \bar{G}_l; a)} \quad (9.1)$$

and, above threshold, the corresponding $S$-matrix element reduces to

$$S_l = (1 + ip_l^2 \mathcal{K}_l)/(1 - ip_l^2 \mathcal{K}_l) \quad (9.2)$$
$$= \exp(2i\delta_l) , \quad (9.3)$$

hence,

$$tg\,\delta_l = \varepsilon_l^2 k_l^{2l+1} \mathcal{K}_l . \quad (9.4)$$

With the definition (2.15) of $I_l, O_l$ neither of the Coulomb phases

$$\sigma_l = \arg\Gamma(l+1+i\eta) , \quad \omega_l = \sigma_l - \sigma_0$$

is included in $\delta_l$. In the expansion

$$\mathcal{K}_l = \sum_\lambda \frac{g_{l\lambda}^2}{E_{l\lambda} - E} , \quad (9.5)$$

we have

$$g_{l\lambda}^2 = \frac{\hbar^2}{2M}[u_l(a, k_{l\lambda})/\bar{G}_l(a, k_{l\lambda})]^2 \nu_{l\lambda}^{-1} \quad (9.6)$$

with

$$\nu_{l\lambda} = \int_0^a u_l^2(r, k_{l\lambda}) dr + \frac{\hbar^2}{2M} u_l^2(a, k_{l\lambda}) \dot{L}_{l\lambda} , \quad (9.7)$$

and from Eqs. (9.4) and (9.5) we easily obtain

$$\left.\frac{d\delta_l}{dE}\right|_{E=E_{l\lambda}} = \frac{1}{p_l^2(E_{l\lambda}) g_{l\lambda}^2} . \quad (9.8)$$

From the latter result, we see that the only real poles $E_{l\lambda}$ associated with a resonance are those for which $g_{l\lambda}^2 > 0$, i.e., $\nu_{l\lambda} > 0$, since only then is the phase shift $\delta_l$ *increasing* through $\pi/2 + (\text{mod } \pi)$ at $E = E_{l\lambda}$. For various square-well potentials, several examples have been given[20] of poles $E_{l\lambda}$ for which $\nu_{l\lambda} < 0$. They are in no way related with a resonance behavior. They parametrize the background part of $\mathcal{K}_l$ which is important for this type of potential. The phase shift is *decreasing* at these energies.

Since the first term of $\nu_{l\lambda}$ in Eq. (9.7) is positive, $\nu_{l\lambda}$ can be negative only when the second term is large and negative. Except for $s$-wave neutrons, this cannot happen at positive energies close to the threshold, because at such energies $\dot{L}_{l\lambda}$ is positive. With $x = (8\alpha a)^{1/2}$, we have

$$(\hbar^2/2M)\dot{L}_{l\lambda} = 2a[xK_{2l+1}^2(x)]^{-2} \times \int_x^\infty K_{2l+1}^2(t) t^3 dt + O(k_{l\lambda}^2) \quad (9.9a)$$

when there is a Coulomb repulsion, and

$$(\hbar^2/2M)\dot{L}_{l\lambda} = a/(2l-1) + O(k_{l\lambda}^2) \quad (9.9b)$$

in the case of a neutron channel. On the contrary, in both cases, at large positive energies, $\dot{L}_{l\lambda}$ is negative, since with $\eta \to 0$, we have

$$(\hbar^2/2M)\dot{L}_{l\lambda} = -\tfrac{1}{2} a k_{l\lambda}^{2l} \bar{G}_{l\lambda}^{-2}[1 + O(k_{l\lambda}^{-1})] \quad (9.10)$$

and $\nu_{l\lambda}$ can then be negative.

The physical interpretation of these results is obvious and it can be extended to the general case of a nuclear reaction proper with $\nu_\lambda$ defined by Eq. (8.4): At the energy of a true resonance, the wave function $\Psi_\lambda$ is very large in the interior region, making the first term of $\nu_\lambda$, which is positive, much larger than the second one which is a surface term. This does not apply when the pole $E_\lambda$ is not associated with a resonance and $\nu_\lambda$ can then be negative. The poles for which $\nu_\lambda < 0$ have been called echo poles, because they are related to the "echoes" analyzed in several papers by McVoy[21] and collaborators. Here, the echo poles contribute to the nonresonant or background part of the $\mathcal{K}$ matrix. To some extent, in the elastic channel, their contribution to the phase shift corresponds

to the hard-sphere phase shift in an $R$-matrix parametrization.

## X. FITTING THE $\mathcal{K}$ MATRIX TO EXPERIMENTAL DATA

A parametrized cross section is obtained from the $S$ matrix derived, by means of the relation (4.12), from the parametrized $\mathcal{K}$-matrix expansion (5.15). In practice, however, fitting the expanded $\mathcal{K}$ matrix to a set of experimental data can only be done over a finite range of energy and using only a few-level approximation of the complete expansion of $\mathcal{K}$. The corresponding $S$-matrix elements are given by

$$S_{dc}=\delta_{dc}+2ip_d\sum_e \mathcal{K}_{de}[(1-i\mu\mathcal{K})^{-1}]_{ec}p_c \ . \tag{10.1}$$

The only elements of $S$ having a physical interest are those with channels $d,c$ both open. Although the sum over $e$ extends, in principle, over all open and closed channels, we have seen in Sec. VII that it suffices to extend it only over the open channels and the closed neutron channels. The modified $\mathcal{K}$ matrix is defined at any energy below, as well as above, any channel threshold. In order to retain the unitarity of $S$, the approximate $\mathcal{K}$ needs only to be real and symmetric.

Accordingly, all the elements of $\mathcal{K}$ used when fitting a set of data should be given the form

$$\mathcal{K}_{dc}=\sum_{\lambda=1}^{\Lambda} g_{d\lambda}g_{c\lambda}/(E_\lambda-E)+B_{dc} \ . \tag{10.2}$$

The finite sum, where $\Lambda$ is never very large, must account for the observed resonances, while $B_{dc}(=B_{cd})$ must account for the nonresonant part of $\mathcal{K}_{dc}$, if any. In particular, $B_{dc}$ can contain an echo pole if this is suggested by the decreasing trend of the phase shift in an elastic channel. $B_{dc}$ can also contain a slowly varying function of the energy to account for the distant levels ($\lambda>\Lambda$) not introduced explicitly into the parametrization.

Recently,[7] in the simultaneous parametrization of the data on $^{12}C(\alpha,\gamma)^{16}O$ and $^{12}C(\alpha,\alpha)^{12}C$, an echo pole plus a linear term in $E$ has been used as a background term of $\mathcal{K}$. But, as it has been done in the $R$-matrix parametrizations[22–25] of the same data, the contribution from distant levels could have been introduced by means of another pole term, with a fixed large energy $E_\lambda$ well above the energy range of the data.

As seen in Sec. VI, the energy of an observed resonance corresponds exactly to the energy of a pole $E_\lambda$ ($\lambda\leq\Lambda$), without shift, except if a closed neutron channel has its threshold just above $E_\lambda$. The reduced width amplitudes $g_{e\lambda}$, associated with a resonance energy $E_\lambda$, have, according to their very definition, a unique value. They are not dependent on the choice of a boundary condition constant. According to Eq. (5.12), $g_{e\lambda}$ is proportional to the *amplitude* ${}^{\mathcal{K}}V_{e\lambda}/\overline{G}_{e\lambda}$ of the "outgoing" wave in channel $e$ at the energy $E_\lambda$.

These properties, together with the unitarity of the corresponding $S$ matrix give the $\mathcal{K}$-matrix analysis of experimental data a good physical basis.

Other applications than the one already published[7] are now projected, including the use of the matrix $\mathcal{M}=\mathcal{K}^{-1}$ in a multichannel effective range expansion at low energy.


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## APPENDIX: THE ENTIRE FUNCTION $\overline{G}_l$

To obtain the entire function $\overline{G}_l$, we have multiplied $G_l$ by $\varepsilon_l k^l$ in order to remove its threshold factor and substituted the polynomial in $\eta^{-2}, h_N(\eta)$ for the singular function $h(\eta)$ defined by Eq. (3.3d)

For $\eta\to\infty$, i.e., $k\to 0$, $h(\eta)$ has the divergent asymptotic expansion[26]

$$h(\eta)\sim\sum_{s=1}^{\infty}\frac{|B_{2s}|}{2s}\eta^{-2s} \ , \tag{A1}$$

where the $B_{2s}$ are the Bernoulli numbers. For a repulsive field ($k\eta=\alpha>0$), its domain of validity is

$$|\arg k|\leq\pi/2-\delta<\pi/2 \tag{A2}$$

(where $\delta$ is arbitrarily small). It does not include the imaginary $k$ axis where $h(\eta)$ has an infinite number of poles.

Using the reflection property of the $\psi$ functions, we obtain

$$\begin{aligned} h^+(\eta)&\equiv h(\eta)+i\pi/(e^{2\pi\eta}-1)\\ &=\psi(i\eta)+\frac{1}{2i\eta}-\ln(e^{i\pi/2}\eta) \ . \end{aligned} \tag{A3}$$

This function $h^+$ also has the asymptotic expansion (A1), but it now holds for

$$|\arg(e^{i\pi/2}\eta)|\leq\pi-\delta<\pi \ .$$

Hence, it holds, in particular, on the positive imaginary $k$ axis and more generally for

$$-\pi/2+\delta\leq\arg k\leq 3\pi/2-\delta \ . \tag{A4}$$

Introducing the notation $\mathcal{E}=\eta^{-2}(\propto E)$, let $H(\mathcal{E})$ be a function defined as follows *for real* $\mathcal{E}$ *only*: $H(\mathcal{E})=h(\eta)$ at *positive energies* ($\mathcal{E}>0$, $\eta>0$), and $H(\mathcal{E})=h^+(\eta)$ at *negative energies* ($\mathcal{E}<0$, $i\eta=\beta>0$). It is then obvious that for *real* energies, the function $H(\mathcal{E})$ for $\mathcal{E}\to\pm 0$ has the divergent asymptotic expansion

$$H(\mathcal{E})\sim\sum_{s=0}^{\infty}\frac{|B_{2s}|}{2s}\mathcal{E}^s \ . \tag{A5}$$

So, despite the fact that both $h(\eta)$ and $h^+(\eta)$ are singular for $\eta\to\infty$, i.e., for $\mathcal{E}=0$, the function $H(\mathcal{E})$ and its derivatives of finite order are defined and continuous for $\mathcal{E}\to+0$ and $\mathcal{E}\to-0$. We have

$$H(0)=0\ ,$$
$$\left.\frac{d^s H(\mathcal{E})}{d\mathcal{E}^s}\right|_{\mathcal{E}=0}=\tfrac{1}{2}(s-1)!|B_{2s}| \quad (1\le s<\infty)\ . \tag{A6}$$

On the real $\mathcal{E}$ axis, $H(\mathcal{E})$ has no other singularity than $\mathcal{E}=0$ for $|\mathcal{E}|<\infty$. Accordingly, from Weierstrass theorem, on any *finite* interval of the real $\mathcal{E}$ axis one can find a polynomial $h_N(\eta)$ of degree $N$ in $\eta^{-2}$, with $N$ sufficiently large, such that

$$|H(\mathcal{E})-h_N(\eta)|\le\varepsilon \tag{A7}$$

for any nonvanishing but arbitrarily small $\varepsilon$. We assume that $\varepsilon$ has been chosen small enough so that on a finite interval $[-\mathcal{E}_0,\mathcal{E}_0]$, with $\mathcal{E}_0>0$, the Eqs. (3.11) are satisfied to this approximation. The fact that, to the same approximation, from Eqs. (3.7) and (2.15), we also have

$$\bar{G}_l=\varepsilon_l k^l G_l \quad (\text{in } c^+)\ , \tag{A8a}$$
$$\bar{G}_l=\varepsilon_l k^l O_l \quad (\text{in } c^-)\ , \tag{A8b}$$

should not be misunderstood: the latter equations are valid numerically, but obviously not analytically. The numerical computation of $h_N(\eta)$ is not required when parametrizing data. The mere existence of $h_N(\eta)$ suffices to justify the $\mathcal{K}$-matrix parametrization derived in Sec. V. The actual computation of $h_N(\eta)$ is required only in order to obtain numerical values of $\bar{G}_l$ at complex energies, since at real energies, positive or negative, numerical values of $\bar{G}_l$ can be obtained from Eqs. (A8). In a closed channel, however, it is useful to rewrite $\varepsilon_l k^l O_l$ in terms of a Whittaker function, namely,[11]

$$\bar{G}_l=(l!)^{-1}b^l\Gamma(l+1+\beta)W_{-\beta,l+1/2}(2br)\ , \tag{A9}$$

where $b=-ik>0$ and $\beta=i\eta=\alpha/b>0$.

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