Multilevel parametrization of resonance neutron cross sections

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The methodological principles of constructing various practical methods for the multilevel parametrization of resonance neutron cross sections are formulated on the basis of the classical results of Wigner R-matrix theory. The general structure of the well known code SAMMY, which has been used effectively in recent years to analyze and represent the detailed energy structure of the cross sections in wide ranges of the region of resolved levels, is discussed. It is shown that similar results can also be obtained by the combined method and the method of rigorous pole expansion of the U matrix. The algorithms for transforming the parameters of the various methods are presented, and their advantages in the practical use of the ENDF/B-6 parameters are discussed. © *1997 American Institute of Physics.* [S1063-7796(97)00104-6]

INTRODUCTION

In the background of the current impressive achievements of nuclear physics such as the discovery of new superheavy elements in reactions involving ions and the discovery of nuclear levels with anomalously large moment (nuclear hyperdeformation), the unusual events occurring in the seemingly quiet area of resonance neutron spectrometry passed unnoticed. The amount and accuracy of the experimental data have grown so much in the last 10 years that the so-called region of unresolved resonances has practically disappeared for many nuclei. The s-wave levels in neutron channels have been augmented by a set of resonances with $l=1,2,\ldots$, interference minima appear quite clearly in the cross sections, and data have been obtained from measurement of the γ spectra in individual resonances, from the interaction of polarized neutrons with oriented nuclei, and so on. For many nuclei the number of experimentally resolved resonances is in the hundreds, and the level parameters and spins and parities have been determined for most of them. In this situation, a consistent analysis and evaluation of the proposed data on the resonance cross sections of various reactions in wide energy ranges requires very general multilevel parametrization methods based on the results of the formal theory of nuclear reactions.[1–5]

The progress made in neutron spectroscopy can be illustrated by the particular example of the recent data on the resonance cross sections of the nuclei of greatest practical importance, ^{235}U and ^{239}Pu, where the region of resolved levels has been extended by almost a factor of 10 (Fig. 1) in recent years.[5,6] The detailed energy structure of these cross sections is reproduced in the ENDF/B-6 nuclear data bank directly by the R-matrix method of parametrization (the SAMMY code).[5,6] Using general kinematical relations, for the total cross section

$$\sigma(E)=2\pi k^{-2}\sum_J g(J)\sum_n \mathrm{Re}[1-U^J_{nn}(E)],$$

the total cross section for neutron absorption (fission and radiative capture)

$$\sigma_a(E)=\pi k^{-2}\sum_J g(J)\sum_n \mathrm{Re}[1-|U^J_{nn}(E)|^2],$$

and the cross section for reaction channel c [in this case, fission channel $c(f)$]

$$\sigma_c(E)=\pi k^{-2}\sum_J g(J)\sum_n \mathrm{Re}|U^J_{cn}(E)|^2, \tag{1}$$

the elements of the collision matrix U^J_{cn} for several fission (c) and neutron (n) channels for each of the possible values of the total angular momentum J and parity are chosen to have the form

$$U^J_{cn}(E)=e^{-i\varphi_c}\left[\frac{2}{1-i\mathbf{K}^J(E)}-1\right]_{cn}e^{-i\varphi_n}, \tag{2}$$

where φ_n is the phase shift and

$$K^J_{c'c}(E)=\frac{1}{2}\sum_{\lambda(J)}\Gamma^{1/2}_{\lambda c'}\Gamma^{1/2}_{\lambda c}/(E_\lambda-E-i\Gamma_{\lambda\gamma}/2) \tag{3}$$

is the analog of the Wigner R matrix with the radiative-capture channels excluded.[1–4] The parameters E_λ, $\Gamma_{\lambda\gamma}$, and $\Gamma_{\lambda c(f)}$ are assumed to be independent of energy, and $\Gamma_{\lambda n}(E)=\Gamma^0_{\lambda n}\sqrt{E}$ (Table I). Here $\Gamma^0_{\lambda n}$ is the reduced neutron width (defined for $l=0$ as $\Gamma^0_{\lambda n}=\Gamma^{\mathrm{res}}_{\lambda n}/\sqrt{E^{\mathrm{res}}_\lambda}$).

The creation and realization of the SAMMY code in the multilevel analysis of resonance cross sections is an important achievement of the ORNL group,[6,7] as it allows the full use of the recent data on the detailed energy structure of the cross sections in applied problems. However, the reproduction of the resonance cross sections using the parameters of the K matrix (3) in general leads to serious computational problems when, for example, the Doppler broadening of resonances is taken into account, or the resonance integrals are found in certain energy ranges. This is a consequence both of the need to include the entire set of level parameters at each step of the integration, and of the complicated matrix form of the energy dependence of the cross sections [the need to invert the matrix $[1-i\mathbf{K}^J(E)]$ in (2)]. In addition, very general analytic properties of the U-matrix elements

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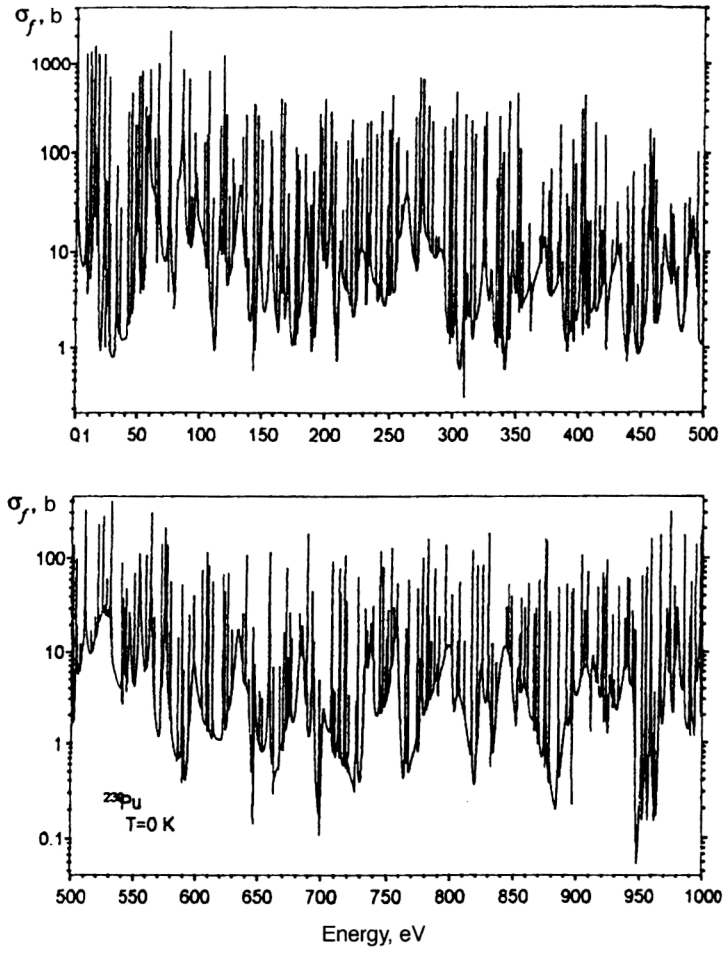

FIG. 1. Fission cross section for ^{239}Pu (ENDF/B-6, Ref. 1).

suggest that it is possible in principle to write them as sums of pole terms in the variable E, or $k=\sqrt{2\mu E}/\hbar$ (Refs. 3 and 8). In this case the resonance cross sections are reproduced as a sum of simple Breit–Wigner terms, which is certainly more convenient for practical applications and does not require a fundamental revision of the existing computational techniques when using the recent data on the resonance structure of the neutron cross sections in the entire range of resolved levels.

A pole form of the collision matrix is characteristic of the Kapur–Peierls[1] and Humblet–Rosenfeld[8] formalisms. Although general schemes for transforming the R-matrix parameters to the parameters of pole expansions are known in principle, their practical realization has become important only very recently with the appearance of new data on the resonance cross sections in broad energy ranges and the results of their multilevel analysis using the SAMMY code.[5,6] Here we review the schemes and methods used for multilevel parametrization of the neutron resonance cross sections and the algorithms for establishing a relationship between the parameters of various schemes. Our practical goal is the construction of multilevel expressions for the cross sections which are mathematically identical to the SAMMY ones and convenient for applications, i.e., expressions which reproduce the real energy structure of the cross sections in the entire range of resolved levels for the corresponding redefinition of the parameters.

1. *R*-MATRIX PARAMETRIZATION METHODS

Here we give the well known relations of Wigner R-matrix theory for the collision matrix $\mathbf{U}(E)$ with elements $U_{c'c}(E)$ and rank equal to the total number of channels effective at the energies of interest. The fundamental unitary representation is[1]

$$U(E)=e^{-i\varphi}\mathbf{P}^{1/2}[1-\mathbf{R}(E)\bar{\mathbf{L}}]^{-1}[1-\mathbf{R}(E)\bar{\mathbf{L}}^*]\mathbf{P}^{-1/2}e^{-i\varphi}, \quad (4)$$

where $\exp(-i\varphi)$ and $\bar{\mathbf{L}}$ are diagonal matrices of the exterior solutions, φ_c is the phase shift of potential scattering, $\bar{L}_c=L_c+b_c$, b_c is the real constant of the boundary condition, and $L_c=S_c+iP_c$ is the logarithmic derivative at the channel radius a_c, the imaginary part of which, P_c, is the penetration factor of the channel c (Appendix 1). The elements of the matrix $\mathbf{R}(E)$ are in general defined as the sum over the complete set of eigenstates in the interior region $(0<r_c<a_c)$ with energies E_λ for fixed value of the total angular momentum J and parity (for now we omit the corresponding indices on $\mathbf{U}$ and $\mathbf{R}$):

$$R_{c'c}=\sum_\lambda \gamma_{\lambda c'}\frac{1}{E_\lambda-E}\gamma_{\lambda c}, \quad (5)$$

where the parameters E_λ and $\gamma_{\lambda c}$ are real constants.[1]

We can also write $R_{c'c}$ (5) as the elements of the channel matrix:

TABLE I. R-matrix parameters of ^{239}Pu.

#	E_λ [eV]	$\Gamma^0_{\lambda n}$ [eV$^{1/2}$]	$\Gamma_{\lambda\gamma}$ [eV$^{1/2}$]	$\Gamma_{\lambda f_1}$ [eV$^{1/2}$]	$\Gamma_{\lambda f_2}$ [eV$^{1/2}$]	J
1	−1.5002E+2	3.5017E−2	4.5720E−2	1.9050E−1	0.0000E−1	1
2	−1.5467E+1	3.4454E−5	2.6850E−2	−2.5530E−6	0.0000E−1	1
3	−6.9087E+0	4.7024E−3	2.6000E−1	−9.4170E−1	2.9620E−1	0
4	−2.1944E−1	6.5045E−5	2.5910E−3	−1.6140E−3	−5.8250E−1	0
5	2.9562E−1	1.4701E−4	3.9300E−2	5.7380E−2	0.0000E−1	1
6	7.8158E+0	2.8329E−4	3.7750E−2	−4.4750E−2	0.0000E−1	1
7	1.0928E+1	5.4299E−4	3.6120E−2	−1.5400E−1	0.0000E−1	1
8	1.1898E+1	2.8269E−4	3.7960E−2	2.0710E−2	0.0000E−1	1
9	1.4329E+1	1.5975E−4	2.9210E−2	5.9040E−2	0.0000E−1	1
10	1.4678E+1	4.9854E−4	3.9160E−2	3.0450E−2	0.0000E−1	1
11	1.5417E+1	5.2567E−4	4.2000E−2	−7.5480E−6	7.5500E−1	0
12	1.7657E+1	4.2908E−4	3.8240E−2	−3.6400E−2	0.0000E−1	1
13	2.2266E+1	5.4846E−4	4.1580E−2	−6.2990E−2	0.0000E−1	1
14	2.3933E+1	1.7522E−5	3.5340E−2	2.5880E−2	0.0000E−1	1
15	2.6269E+1	3.0105E−4	3.9040E−2	4.1120E−2	0.0000E−1	1
16	2.7288E+1	2.8581E−5	3.8710E−2	2.7880E−3	0.0000E−1	1
17	3.2327E+1	1.5310E−4	4.2520E−2	8.1710E−3	−1.2790E−1	0
18	3.5486E+1	4.5291E−5	4.0920E−2	3.5470E−3	0.0000E−1	1
19	4.1457E+1	5.1315E−4	4.8930E−2	−6.4090E−3	0.0000E−1	1
20	4.1736E+1	1.4473E−4	3.7700E−2	6.1030E−2	0.0000E−1	1
21	4.4531E+1	9.1891E−4	4.0030E−2	−4.3730E−3	0.0000E−1	1
22	4.7534E+1	7.0186E−4	3.1460E−2	4.8150E−1	−1.2740E−7	0
23	4.9576E+1	6.0730E−4	4.2000E−2	−1.0490E+0	4.9830E−3	0
24	5.0144E+1	4.5952E−4	2.2500E−2	−4.9960E−3	0.0000E−1	1
25	5.2648E+1	1.3038E−3	4.3940E−2	−9.0450E−3	0.0000E−1	1
26	5.5704E+1	2.0205E−4	3.7560E−2	2.4270E−2	0.0000E−1	1
27	5.6924E+1	1.5666E−3	4.2000E−2	−2.2040E+0	2.5300E−2	0
28	5.9291E+1	5.7727E−4	3.3900E−2	9.8690E−2	0.0000E−1	1
29	6.1621E+1	3.5835E−3	4.2000E−2	7.0980E+0	6.6790E−3	0
30	6.3170E+1	7.9190E−5	3.5270E−2	7.2420E−2	0.0000E−1	1
31	6.5454E+1	4.6537E−4	2.4110E−2	4.5020E−1	−2.1170E−9	0
32	6.5793E+1	1.1948E−3	6.1610E−2	1.0910E−1	0.0000E−1	1
33	7.4167E+1	3.7285E−4	3.1210E−2	−2.9710E−2	0.0000E−1	1
34	7.4885E+1	3.0346E−4	4.2000E−2	1.2530E−3	−3.4030E−1	0
35	7.5034E+1	2.4116E−3	4.0160E−2	−8.9020E−2	0.0000E−1	1
36	7.9085E+1	4.8263E−6	4.1820E−2	6.1800E−3	0.0000E−1	1
37	8.0872E+1	5.0095E−4	4.2000E−2	1.8600E+0	−1.7600E−3	0
38	8.2774E+1	3.6404E−5	4.6850E−2	5.1500E−3	0.0000E−1	1
39	8.5507E+1	5.3974E−3	5.1000E−2	−1.8440E+0	3.0440E−3	0
40	8.5618E+1	8.8555E−4	2.6180E−2	5.8660E−3	0.0000E−1	1
41	9.0850E+1	1.2810E−3	3.3990E−2	7.3610E−3	0.0000E−1	1
42	9.3079E+1	6.9965E−5	3.7640E−2	−2.8980E−3	0.0000E−1	1
	.....	.....	.....	.....	.....	.
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400	9.9424E+2	5.9972E−4	4.3060E−2	3.2550E−2	0.0000E−1	1
401	9.9797E+2	1.1256E−3	3.1420E−2	−2.7140E−1	0.0000E−1	1
402	9.9867E+2	1.1167E−3	3.9660E−2	−4.0760E−2	0.0000E−1	1
403	1.0050E+3	2.4361E−3	4.6000E−2	1.1950E−3	0.0000E−1	1
404	1.0100E+3	5.8243E−3	4.6000E−2	−4.9200E+0	2.0850E−2	0
405	1.1000E+3	3.6784E−2	4.6000E−2	4.2000E−2	0.0000E−1	1

Note: The ± of $\Gamma_{\lambda f}$ corresponds to the sign of the product $(\Gamma^0_{\lambda n})^{1/2}\Gamma^{1/2}_{\lambda f_i}$.

$$\mathbf{R}(E)=\boldsymbol{\gamma}^{\mathrm{T}}\frac{1}{\mathscr{E}-E}\,\boldsymbol{\gamma}, \tag{6}$$

where $\mathscr{E}$ is the diagonal level matrix with elements E_λ, and $\boldsymbol{\gamma}$ is a rectangular matrix ($\lambda\times c$) with elements $\gamma_{\lambda c}$ ($\boldsymbol{\gamma}^{\mathrm{T}}$ is the transpose). We also introduce the matrix

$$\mathbf{G}=(\mathbf{1}-\mathbf{R}\bar{\mathbf{L}})^{-1}\mathbf{R}\quad(\mathbf{G}=\mathbf{R}+\mathbf{R}\bar{\mathbf{L}}\mathbf{G}), \tag{7}$$

and if we define

$$\mathbf{G}=\boldsymbol{\gamma}^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\gamma}, \tag{8}$$

from Eq. (7) we find the level matrix $\mathbf{A}$:

$$\mathbf{A}=\mathscr{E}-\mathbf{E}-\boldsymbol{\gamma}\bar{\mathbf{L}}\boldsymbol{\gamma}^{T},\quad A_{\lambda\mu}=(E_\lambda-E)\delta_{\lambda\mu}-\xi_{\lambda\mu}, \tag{9}$$

where

$$\xi_{\lambda\mu}=(\boldsymbol{\gamma}\bar{\mathbf{L}}\boldsymbol{\gamma}^{\mathrm{T}})_{\lambda\mu}=\Delta_{\lambda\mu}+i\Gamma_{\lambda\mu}/2=\sum_c\gamma_{\lambda c}(S_c-b_c)\gamma_{\mu c}$$

$$+i\sum_c \gamma_{\lambda c}P_c\gamma_{\mu c}.$$

As a result, we obtain an alternative representation for $\mathbf{U}(E)$ (4) in terms of the level matrix $\mathbf{A}$ (Ref. 1):

$$\mathbf{U}(E)=e^{-i\varphi}[1+2i\mathbf{P}^{1/2}\mathbf{G}\mathbf{P}^{1/2}]e^{-i\varphi}$$
$$=e^{-i\varphi}[1+2i\mathbf{P}^{1/2}\boldsymbol{\gamma}^{T}\mathbf{A}^{-1}\boldsymbol{\gamma}\mathbf{P}^{1/2}]e^{-i\varphi} \quad (10)$$

or

$$U_{cn}(E)=e^{-i\varphi_c}\Big[\delta_{cn}$$
$$+2iP_c^{1/2}\sum_{\lambda\mu}\gamma_{\lambda c}\gamma_{\mu n}(A^{-1})_{\lambda\mu}P_n^{1/2}\Big]e^{-i\varphi_n} \quad (11)$$

(in the review of Ref. 1 the inverse $\mathbf{A}^{-1}$ is used for $\mathbf{A}$).

For over 40 years, these two identical forms of the matrix $\mathbf{U}(E)$, (4) and (11), determined by Wigner R-matrix theory have served as the methodological basis for constructing various practical schemes of parametrizing the resonance cross sections and physically analyzing the parameters. Of course, the most popular approximation is the one-level one (the Breit–Wigner formula) used to describe the energy dependence of the cross sections at isolated resonances. The parameters defined here, the level energies E_λ and the resonance widths of individual channels $\Gamma_{\lambda c}$, have a qualitative interpretation in microscopic interaction models.[1–3,9] The statistical distributions of the values of these parameters are known, and there are standardized procedures for including the Doppler broadening of resonances, averaging the cross sections over energy, and analyzing the data on resonance-neutron transmission. The one-level approximation is also used in the theory and methods of neutron-physics calculations for nuclear reactors.[10]

However, the two-level approximation for the case of two closely spaced resonances [$\lambda=1,2$ in the R matrix (5)] illustrates the effect of interference, which tends to increase or decrease the cross sections in relation to the simple sum of one-level expressions. And sometimes it is also possible for fictitious resonances to appear when there is nonresonance background.[3–5] In practice, the inclusion of level interference is most important for the resonance cross sections of fissile nuclei. Therefore, the problems of multilevel parametrization are mainly concentrated in applications to fissile elements, although in recent years the R-matrix analysis has also been used effectively to analyze the resonance cross sections of nonfissile nuclei.[7,11]

Obviously, when the number of reaction channels is large, the direct use of the R-matrix relations (4) and (11) in a multilevel analysis is very problematical, owing to the absence of a complete set of data on each of the channels and an abundance of free parameters. Certain physical assumptions are needed to simplify the analysis. The most effective one has proved to be the Reich–Moore (RM) approximation, where the number of channels for neutron radiative capture is assumed to be large with a random (Gaussian) distribution of the corresponding amplitudes $\gamma_{\lambda c}$, so that

$$2\sum_{c(\gamma)}\gamma_{\lambda c}P_c\gamma_{\mu c}\approx\Gamma_{\lambda\gamma}\delta_{\lambda\mu}. \quad (12)$$

The error of the RM approximation is determined from the smallness of the ratio

$$\sum_{c(\gamma)}\gamma_{\lambda c}P_c\gamma_{\mu c}/(E_\lambda-E_\mu)\ll 1 \quad (\lambda\neq\mu),$$

which apparently is always satisfied in practice. At least, up to now no effects related to the limitation of the RM approximation have been seen in multilevel parametrization of the cross sections. The use of this approximation greatly decreases the number of channels explicitly included in the analysis, and in the expressions for the cross sections (1) it becomes possible to transform to the reduced collision matrix $\mathbf{U}'(E)$, with rank equal to the number of channels (neutron and fission in our applications) remaining after radiative capture is excluded. It differs from $\mathbf{U}(E)$ (11) by the choice of the level matrix $\mathbf{A}$ (9) in the form

$$A_{\lambda\mu}=(E_\lambda-E-i\Gamma_{\lambda\gamma}/2)\delta_{\lambda\mu}-\xi'_{\lambda\mu}, \quad (13)$$

where

$$\xi'_{\lambda\mu}=\sum_c{}' \gamma_{\lambda c}\bar{L}_c\gamma_{\mu c}=\Delta'_{\lambda\mu}+i\sum_c{}' \gamma_{\lambda c}P_c\gamma_{\mu c}$$

is the sum over the other channels. In the corresponding fundamental representation of the matrix $\mathbf{U}'(E)$ (4) the elements of the reduced R matrix are defined as

$$R'_{c'c}=\sum_\lambda \gamma_{\lambda c'}\frac{1}{E_\lambda-E-i\Gamma_{\lambda\gamma}/2}\gamma_{\lambda c}. \quad (14)$$

In contrast to $\mathbf{U}(E)$ (4), the reduced matrix $\mathbf{U}'(E)$ is not unitary, and if the total, absorption, and fission cross sections are defined as in the general case by the elements $U'_{nn}(E)$ and $U'_{cn}(E)$ (1), then the cross section for radiative capture is found from the condition of unitarity in all the channels of the matrix $\mathbf{U}(E)$ (4):

$$\sigma_\gamma\sim\sum_{c(\gamma)}|U_{cn}|^2=1-\sum_c{}'|U'_{cn}|^2.$$

The other approximation of the SAMMY code, that the penetration factors for the fission channels and, accordingly, the fission widths are independent of energy, is less obvious. The main argument for this is only that the region of resolved resonances is limited to an interval of ~ 1 keV, while the penetration factors for fission are functions of the difference $E-E_{\text{th}}$, where the barrier energy E_{th} is on the MeV scale.[2]

Finally, neglect of the level-shift factor $\Delta'_{\lambda\mu}$ (13) in the collision matrix (2), which is obvious for neutron channels with $l=0$, is apparently also allowed for $l\geq 1$ at energies below the inelastic neutron scattering threshold, given the phenomenological nature of the resonance parameters of the code.

It should be noted that in the SAMMY code the sum over $\lambda(J)$ (3) contains an arbitrarily large but finite number of terms $N(J)$. Therefore, here there is no need to formally isolate the background (nonresonance) part of the $\mathbf{K}(E)$ matrix, as was usually done in early R-matrix parametrization

schemes.[1,3] In fact, the existing background is taken into account by the corresponding extension of the sum (3) to both positive and negative values of E_λ, instead of the resonances actually observed in the energy range of interest.

When applied to nonfissile nuclei, this R-matrix parametrization scheme looks simpler. For example, in a typical case involving a single neutron channel, for a system of levels with given J and parity the total cross section and the neutron absorption cross section can be written as ratios of sums:[3]

$$\sigma(E)=4\pi k^{-2}\sum_J g(J)\left[\sin^2\varphi_n + \mathrm{Re}\left(e^{-2i\varphi_n}\frac{-iK^J_{nn}(E)}{1-iK^J_{nn}(E)}\right)\right],$$

$$\sigma_a(E)=4\pi k^{-2}\sum_J g(J)\mathrm{Re}\left(\frac{-iK^J_{nn}(E)}{|1-iK^J_{nn}(E)|^2}\right), \qquad (15)$$

where

$$K^J_{nn}(E)=\frac{1}{2}\sum_{\lambda(J)}\Gamma_{\lambda n}(E)/(E_\lambda-E-i\Gamma_{\lambda\gamma}/2).$$

Here the parameters $\Gamma_{\lambda n}(E_\lambda)$, $\Gamma_{\lambda\gamma}$, and E_λ have the same physical meaning as in the one-level approximation. A similar functional dependence on the energy in the form of a ratio of sums of pole terms is obtained by direct inversion of the matrix $[1-i\mathbf{K}^J(E)]$ (2) for two or more neutron channels (see Sec. 6).

2. THE ADLER METHOD

Another classical version of the resonance $\mathbf{U}(E)$ matrix is given by the Kapur–Peierls formalism.[1] The corresponding transformation of the R-matrix expression (11) is usually illustrated as the result of diagonalization of the symmetric level matrix $\mathbf{A}$ (9) by an orthogonal complex transformation:[1,12]

$$\mathbf{VAV}^{\mathrm{T}}=\tilde{\mathscr{E}}-\mathbf{E},\quad \mathbf{A}^{-1}=\mathbf{V}^{\mathrm{T}}(\tilde{\mathscr{E}}-\mathbf{E})^{-1}\mathbf{V}\quad(\mathbf{VV}^{\mathrm{T}}=1), \qquad (16)$$

where $\mathbf{V}$ is the transformation matrix and $\tilde{\mathscr{E}}$ is the diagonal level matrix with elements $\tilde{E}_k=\mu_k-i\nu_k$. The resulting expression for $\mathbf{U}(E)$ is

$$\mathbf{U}(E)=e^{-i\boldsymbol{\varphi}}[1+2i\mathbf{P}^{1/2}\tilde{\boldsymbol{\gamma}}^{\mathrm{T}}(\tilde{\mathscr{E}}-\mathbf{E})^{-1}\tilde{\boldsymbol{\gamma}}\mathbf{P}^{1/2}]e^{-i\boldsymbol{\varphi}},$$

$$\tilde{\boldsymbol{\gamma}}=\mathbf{V}\boldsymbol{\gamma},$$

or

$$U_{cn}(E)=e^{-i\varphi_c}\left[\delta_{cn}+2iP_c^{1/2}P_n^{1/2}\sum_k \tilde{\gamma}_{kc}\tilde{\gamma}_{kn}(\tilde{E}_k-E)^{-1}\right]e^{-i\varphi_n}, \qquad (17)$$

where the parameters $\tilde{\gamma}_{kc}$ and $\tilde{E}_k$ are complex and in general depend on the energy.[1–4]

In contrast to R-matrix methods of parametrization, where the resonance cross sections are in general represented as complex functions of the energy in a form that depends on the number of terms in the sums over λ, the Kapur–Peierls formalism appears more convenient for applications, because the cross sections are written as sums of similar one-level terms (see below). However, as already noted, the parameters of the formalism depend on energy, though this dependence may be unimportant, since it is related only to the component $\xi'_{\lambda\mu}$ (13) pertaining to neutron channels. Therefore, when applied to fissile nuclei, where $\Gamma_{\lambda f}+\Gamma_{\lambda\gamma}\gg\Gamma_{\lambda n}$, in diagonalizing the level matrix $\mathbf{A}$ (13) it is possible to take

$$\sum_n \gamma_{\lambda n}\bar{L}_n(E)\gamma_{\mu n}\approx i/2\sum_n \Gamma^{1/2}_{\lambda n}(E_\lambda)\Gamma^{1/2}_{\mu n}(E_\mu),$$

and then the transformation matrix $\mathbf{V}$ and the complex parameters $\tilde{E}_k=\mu_k-i\nu_k$ and $\tilde{\gamma}_{kc}$ no longer depend on energy. The corresponding version of the Kapur–Peierls formalism as applied to the parametrization of resonance cross sections is known as the Adler (AA) method.[5,13]

Substituting $U_{cn}(E)$ (17) into the expression for the cross sections (1), we obtain the multilevel expressions of the AA method:

$$\sigma(E)=\sigma_p+4\pi k^{-2}\sum_J g(J)\sum_n P_n(E)\times\sum_k \mathrm{Re}\left[(-i)e^{-2i\varphi_n}\frac{g_k+ih_k}{\mu_k-E-i\nu_k}\right], \qquad (18)$$

where $g_k+ih_k=\tilde{\gamma}^2_{kn}$, σ_p is the potential cross section, and

$$\sigma_c(E)=4\pi k^{-2}\sum_J g(J)\sum_n P_n(E)\times\sum_k \mathrm{Re}\left[(-i)\frac{g^c_k+ih^c_k}{\mu_k-E-i\nu_k}\right], \qquad (19)$$

with

$$g^c_k+ih^c_k=2iP_c\sum_{k'}\frac{\tilde{\gamma}_{kn}\tilde{\gamma}_{kc}\tilde{\gamma}^*_{k'n}\tilde{\gamma}^*_{k'c}}{(\mu_{k'}-\mu_k)+i(\nu_{k'}+\nu_k)}. \qquad (20)$$

These are obviously sums of typical Breit–Wigner terms with parameters g_k, h_k, g^c_k, h^c_k, μ_k, and ν_k independent of energy in the AA method. In applications to fissile nuclei only one neutron channel with $l=0$ ($P_n=P_0=ka$) is usually considered, and then the cross sections can be written as[5,13]

$$\sigma(E)=\sigma_p+\frac{1}{\sqrt{E}}\sum_k \mathrm{Re}\left[(-i)e^{-2i\varphi_0}\frac{G_k+iH_k}{\mu_k-E-i\nu_k}\right],$$

$$\sigma_f(E)=\frac{1}{\sqrt{E}}\sum_k\frac{G^f_k\nu_k+H^f_k(\mu_k-E)}{(\mu_k-E)^2+\nu_k^2}, \qquad (21)$$

with parameters independent of energy:

$$G_k+iH_k=(4\pi a\hbar/\sqrt{2\mu})g(J)(g_k+ih_k),$$

$$G^f_k+iH^f_k=(4\pi a\hbar/\sqrt{2\mu})g(J)\sum_{c(f)}(g^c_k+ih^c_k).$$

This representation of the resonance cross sections of fissile nuclei is also used in the ENDF library.[5]

Equations (18)–(21) are undoubtedly more convenient for applications, because for an arbitrary number of levels they have a single type of energy structure which is directly associated with observable resonances. However, when the parameters of the AA method are chosen independently, it is possible for paradoxical "negative" cross sections to arise, owing to the fact that the H components have variable sign.[14] Therefore, in practice, for a restricted number of resonance terms it is common to add to the sums (18)–(21) a background term due to the tails of the remaining levels which cancels negative values. This results in the appearance of additional background parameters in the individual energy ranges.[5,13]

Actually, the parameters of the Kapur–Peierls formalism cannot be considered independent, because there is a relation between them due to the unitarity condition on the $\mathbf{U}(E)$ matrix (17). In contrast to R-matrix schemes, where the expression used for $\mathbf{U}(E)$ (4) is unitary for any choice of independent parameters, for the pole representation (17) this condition leads to the relation[13,14] (see Appendix 2)

$$\tilde{\gamma}_{kn}^2=2i\sum_c P_c\sum_{k'(J)}\frac{\tilde{\gamma}_{kn}\tilde{\gamma}_{kc}\tilde{\gamma}_{k'n}^*\tilde{\gamma}_{k'c}^*}{\tilde{E}_{k'}^*-\tilde{E}_k}=\sum_c (g_k^c+ih_k^c), \tag{22}$$

where the sum over c includes all the relevant channels, including radiative ones. In particular, it follows from it that in the total absorption cross section determined as in (19) by a sum over channels $c\neq n$,

$$\sigma_a(E)=4\pi k^{-2}\sum_J g(J)\sum_n P_n(E)\times\sum_k \mathrm{Re}\left[(-i)\frac{g_k^a+ih_k^a}{\mu_k-E-i\nu_k}\right],$$

the parameters are

$$g_k^a+ih_k^a=\tilde{\gamma}_{kn}^2-\sum_n (g_k^n+ih_k^n). \tag{23}$$

Then, if analysis of the total cross section (for example, for the case of a single neutron channel) gives $\tilde{\gamma}_{kn}^2$ together with μ_k and ν_k, this is sufficient for finding the parameters $g_k^a+ih_k^a$ (23) and constructing the resonance cross section $\sigma_a(E)$. Here the cross section for radiative capture is obtained as the difference $\sigma_\gamma(E)=\sigma_a(E)-\sigma_f(E)$, and the scattering cross section is $\sigma_n(E)=\sigma(E)-\sigma_a(E)$ (Ref. 14).

The R-matrix parameters can easily be transformed to the parameters of the Adler method, which amounts to diagonalization of the level matrix $\mathbf{A}$ (13), by finding the orthogonal transformation matrix $\mathbf{V}$ by direct inversion, as is done in the POLLA program.[15] In fact, if the usual definition of the elements of the inverse matrix is used,

$$(A^{-1})_{\lambda\mu}=M_{\lambda\mu}(E)/D(E), \tag{24}$$

where $D(E)$ is the determinant and $M_{\lambda\mu}(E)$ is the cofactor of the matrix $\mathbf{A}$, then the determinant is a polynomial in E of degree N equal to the rank of the matrix (the number of levels). Determining the N roots of this polynomial E_k by the Newton–Raphson method, for example, we write

$$D(E)=\prod_{k=1}^N (\tilde{E}_k-E). \tag{25}$$

Here the cofactors are also polynomials in E of degree $N-1$ for the diagonal terms and $N-2$ for the off-diagonal ones. If we assume that all N roots of the determinant are different (nondegenerate), we can write the ratio of polynomials (24) as an expansion in simple fractions:

$$(A^{-1})_{\lambda\mu}=\sum_{k=1}^N \frac{m_{\lambda\mu}(\tilde{E}_k)}{\tilde{E}_k-E}, \tag{26}$$

where

$$m_{\lambda\mu}(\tilde{E}_k)=-M_{\lambda\mu}(\tilde{E}_k)/D'(\tilde{E}_k).$$

Substitution of (26) into the expression for the $\mathbf{U}(E)$ matrix (11) leads directly to the pole form (17) with

$$\tilde{\gamma}_{kn}\tilde{\gamma}_{kc}=\sum_{\lambda\mu}\gamma_{\lambda n}m_{\lambda\mu}(\tilde{E}_k)\gamma_{\mu c}. \tag{27}$$

This transformation method is formally equivalent to diagonalization of the level matrix $\mathbf{A}$ by the orthogonal transformation (16) (Refs. 12 and 15).

The inverse problem of finding the R-matrix parameters from the given parameters of the AA method is in general nonunique both from the mathematical point of view, and owing to the approximations of the method itself.

3. THE COMBINED METHOD

While the scheme of parametric representation of the resonance cross sections discussed above appears attractive, it is obviously limited to relatively small energy ranges, where the variation of the logarithmic derivatives of the neutron channels can be neglected. When the region of resolved levels is extended, this makes it necessary to correct the parameters accordingly in going from one range to another. Meanwhile, as noted above, the very idea of reproducing resonance cross sections as sums of one-level terms follows from the general analytic properties of the $\mathbf{U}(E)$ matrix. Below in Sec. 5 we shall return to the problem of justifying the pole expansion of the $\mathbf{U}(E)$ matrix by a method more rigorous than in the AA method, but first we consider the results of the combined method of multilevel parametrization, which seem mathematically and physically clear. Here the functional dependence of the cross sections on energy is represented as a ratio of sums of pole terms in E as in (15).

In principle, the results of this method follow from the well known Teichmann–Wigner procedure for excluding reaction channels in the $\mathbf{U}(E)$ matrix.[1] Here we shall present a more compact derivation using the matrix relations for $\mathbf{G}(E)$ in (7) and (8). We split the entire set of channels included in the analysis into two groups n, which in our case are neutron channels, and a, which are reaction channels including radiative ones. Accordingly, we represent the rectangular matrix $\boldsymbol{\gamma}$ as two blocks: the $(\boldsymbol{\lambda}\times\mathbf{n})$ block $\boldsymbol{\gamma}_n$ with the number of columns equal to the number of neutron channels and the $(\boldsymbol{\lambda}\times\mathbf{a})$ block $\boldsymbol{\gamma}_a$ for the channels of group a. We also use the matrix identity (9):

$$\mathbf{A}^{-1}=\frac{1}{\mathscr{E}-\mathbf{E}-\boldsymbol{\gamma}\bar{\mathbf{L}}\boldsymbol{\gamma}^{\mathrm{T}}}=\frac{1}{\mathscr{E}-\mathbf{E}-\boldsymbol{\gamma}_a\bar{\mathbf{L}}_a\boldsymbol{\gamma}_a^{\mathrm{T}}}\left[1\right.$$

$$\left.+\boldsymbol{\gamma}_n\bar{\mathbf{L}}_n\boldsymbol{\gamma}_n^{\mathrm{T}}\frac{1}{\mathscr{E}-\mathbf{E}-\boldsymbol{\gamma}\bar{\mathbf{L}}\boldsymbol{\gamma}^{\mathrm{T}}}\right], \tag{28}$$

where

$$(\boldsymbol{\gamma}_a\bar{\mathbf{L}}_a\boldsymbol{\gamma}_a^{\mathrm{T}})_{\lambda\mu}=\sum_{c(a)}\gamma_{\lambda c}\bar{L}_c\gamma_{\mu c},$$

$$(\boldsymbol{\gamma}_n\bar{\mathbf{L}}_n\boldsymbol{\gamma}_n^{\mathrm{T}})_{\lambda\mu}=\sum_{c(n)}\gamma_{\lambda c}\bar{L}_c\gamma_{\mu c}$$

are the scalar products for each group of channels. Multiplying on the right and left by the corresponding matrices $\boldsymbol{\gamma}_a$ or $\boldsymbol{\gamma}_n$, we obtain the matrix relations

$$\mathbf{G}_{nn}=\boldsymbol{\gamma}_n^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\gamma}_n=\mathscr{R}_{nn}+\mathscr{R}_{nn}\bar{\mathbf{L}}_n\mathbf{G}_{nn},$$

$$\mathbf{G}_{an}=\boldsymbol{\gamma}_a^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\gamma}_n=\mathscr{R}_{an}+\mathscr{R}_{an}\bar{\mathbf{L}}_n\mathbf{G}_{nn},$$

$$\mathbf{G}_{aa}=\boldsymbol{\gamma}_a^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\gamma}_a=\mathscr{R}_{aa}+\mathscr{R}_{an}\bar{\mathbf{L}}_n\mathbf{G}_{na}, \tag{29}$$

where

$$\mathscr{R}_{nn}=\boldsymbol{\gamma}_n^{\mathrm{T}}B^{-1}\boldsymbol{\gamma}_n,\quad \mathscr{R}_{an}=\boldsymbol{\gamma}_a^{\mathrm{T}}B^{-1}\boldsymbol{\gamma}_n,\quad \mathscr{R}_{aa}=\boldsymbol{\gamma}_a^{\mathrm{T}}B^{-1}\boldsymbol{\gamma}_a \tag{30}$$

are the blocks of the reduced R matrix with elements

$$\mathscr{R}_{c'c}=\sum_{\lambda\mu}\gamma_{\lambda c'}(B^{-1})_{\lambda\mu}\gamma_{\mu c} \tag{31}$$

and the level matrix

$$\mathbf{B}=\mathscr{E}-\mathbf{E}-\boldsymbol{\gamma}_a\bar{\mathbf{L}}_a\boldsymbol{\gamma}_a^{\mathrm{T}},\quad B_{\lambda\mu}=(E_\lambda-E)\delta_{\lambda\mu}$$

$$-\sum_{c\neq n}\gamma_{\lambda c}\bar{L}_c\gamma_{\mu c}. \tag{32}$$

In contrast to **A** (9), the matrix **B** does not contain neutron channels, and its nondiagonal part $\boldsymbol{\gamma}_a\bar{\mathbf{L}}_a\boldsymbol{\gamma}_a^{\mathrm{T}}$ is assumed to be independent of the energy E. Then the result of diagonalizing **B** by an orthogonal complex transformation (16), for example, leads to the pole expansion of the reduced R matrix,

$$\mathscr{R}_{c'c}=\sum_q\bar{\gamma}_{qc'}\bar{\gamma}_{qc}/(\bar{E}_q-E), \tag{33}$$

with complex parameters $\bar{\gamma}_{qc}$ and $\bar{E}_q$ independent of energy:

$$\bar{\gamma}_{qc}=\sum_\lambda V_{q\lambda}\gamma_{\lambda c},\quad \bar{E}_q=\sum_\lambda V_{q\lambda}^2E_\lambda$$

$$-\sum_{\lambda\mu}V_{q\lambda}(\gamma_a\bar{L}_a\gamma_a^{\mathrm{T}})_{\lambda\mu}V_{q\mu}.$$

(The transformation matrix **V** here is different from that used to diagonalize **A** (16), and so the parameters are also different from those in Sec. 2.)

For nonfissile nuclei the elements of the reduced matrix (31) in the RM approximation coincide with $R'_{c'c}(E)$ (13), and, setting $\mathrm{Re}\,\bar{L}_n=0$, we immediately arrive at the SAMMY scheme with the cross sections in the form of ratios of sums of pole terms (15). We shall show that the expressions for the cross sections in the case of fissile nuclei also transform to a similar form. From (29) we find

$$\mathbf{G}_{nn}=\mathscr{R}_{nn}(1-\bar{\mathbf{L}}_n\mathscr{R}_{nn})^{-1},\quad \mathbf{G}_{an}=\mathscr{R}_{an}(1-\bar{\mathbf{L}}_n\mathscr{R}_{nn})^{-1}, \tag{34}$$

and in the case of, for example, one neutron channel and an arbitrary number of reaction channels the elements of the collision matrix (10) are written in functional form as

$$U_{cn}(E)=\mathrm{e}^{-i\varphi_c}\left[\delta_{cn}\right.$$

$$\left.+2iP_c^{1/2}\frac{\mathscr{R}_{cn}(E)}{1-\bar{L}_n(E)\mathscr{R}_{nn}(E)}P_n^{1/2}\right]\mathrm{e}^{-i\varphi_n}. \tag{35}$$

The expressions for the total cross section and for the neutron absorption cross section are similar to (15):

$$\sigma(E)=4\pi k^{-2}\sum_J g(J)\left[\sin^2\varphi_n\right.$$

$$\left.+\mathrm{Re}\left(\mathrm{e}^{-2i\varphi_n}\frac{-iP_n(E)\mathscr{R}_{nn}^J(E)}{1-\bar{L}_n(E)\mathscr{R}_{nn}^J(E)}\right)\right],$$

$$\sigma_a(E)=4\pi k^{-2}\sum_J g(J)P_n(E)\,\mathrm{Im}\,\mathscr{R}_{nn}^J(E)/|1$$

$$-\bar{L}_n(E)\mathscr{R}_{nn}^J(E)|^2, \tag{36}$$

and the cross section for a reaction in a channel $c\neq n$ is

$$\sigma_c(E)=4\pi k^{-2}\sum_J g(J)\frac{P_cP_n|\mathscr{R}_{cn}^J(E)|^2}{|1-\bar{L}_n(E)\mathscr{R}_{nn}^J(E)|^2}$$

$$=4\pi k^{-2}\sum_J\frac{g(J)P_n(E)}{|1-\bar{L}_n(E)\mathscr{R}_{nn}^J(E)|^2}$$

$$\times\mathrm{Re}(-i)\sum_{q(J)}\frac{\bar{g}_q^c+i\bar{h}_q^c}{\bar{E}_q-E}, \tag{37}$$

where

$$\bar{g}_q^c+i\bar{h}_q^c=2iP_c\sum_{q'}\frac{\bar{\gamma}_{qn}\bar{\gamma}_{qc}\bar{\gamma}_{q'n}^*\bar{\gamma}_{q'c}^*}{\bar{E}_{q'}^*-\bar{E}_q} \tag{38}$$

are complex constants [if $P_c(E)=\mathrm{const}$]. The cross sections for fission and radiative capture summed over their channels are also written in a form similar to (37) with

$$\bar{g}_q^f+i\bar{h}_q^f=\sum_{c(f)}(\bar{g}_q^c+i\bar{h}_q^c),\quad \bar{g}_q^\gamma+i\bar{h}_q^\gamma=\sum_{c(\gamma)}(\bar{g}_q^c+i\bar{h}_q^c). \tag{39}$$

In the combined method the unitarity condition for the collision matrix reduces to relations between the elements

$$\mathrm{Im}\,\mathscr{R}_{nn}^J=\sum_{c\neq n}P_c|\mathscr{R}_{cn}^J|^2 \tag{40}$$

and the parameters of the combined method (Appendix 2),

$$\bar{\gamma}_{qn}^2=\bar{g}_q^f+i\bar{h}_q^f+\bar{g}_q^\gamma+i\bar{h}_q^\gamma, \tag{41}$$

so that to parametrize the cross sections here it is sufficient to determine the set of complex constants $\bar{E}_q$, $\bar{\gamma}_{qn}^2$, and $g_q^f+i\bar{h}_q^f$ for all q.

We see that this method of multilevel parametrization represents a combination of the transformation from R-matrix theory of the **U** (or **G**) matrix to block form (the Teichmann–Wigner method) and the procedure of diagonalization of the level matrix in the reduced R matrix (33). The fact that, in contrast to the AA method, the parameters $\bar{\gamma}_{qc}$ and $\bar{E}_q$ here are independent of energy [if $\bar{L}_c(E)=\text{const}$ for $c\neq n$] ensures that the results of the multilevel parameterization in the combined method and the SAMMY scheme are formally identical (see Sec. 4).

In problems involving two or more neutron channels, the representation of the cross sections as ratios of sums characteristic of the combined method is preserved, because the determinant of the matrix $(\mathbf{1}-\mathbf{L}_n\mathscr{R}_{nn})$ and the elements of the blocks $\mathbf{G}_{nn}$ and $\mathbf{G}_{an}$ (34) are transformed to a form similar to the one-channel variant with the parameters redefined accordingly (Sec. 6 and Appendix 3).

The general formulation of the combined method does not involve any restrictions on either the number of fission channels or the number of radiative capture channels (the RM approximation is certainly not required). In addition, the level-shift factor is taken into account explicitly, which is important near the inelastic-scattering threshold (Sec. 6). Therefore, the parametrization is more universal than that in the SAMMY scheme.

4. THE PARAMETERS OF THE COMBINED METHOD

The algorithms of R-matrix methods of multilevel analysis of the cross sections of nonfissile nuclei[3,7,11] can serve as the basis for constructing a scheme for the independent determination of the parameters of the combined method from analysis of data on the resonance cross sections of fissile nuclei, because the general structure of the representation of the energy dependence (15) and (36), (37) is similar in many respects. Analysis of the total cross section and of the absorption cross section (36) gives the parameters $\mathscr{R}_{nn}(E)-\bar{\gamma}_{qn}^2$ and $\bar{E}_q$, and the data on the fission cross section determine $\bar{g}_q^f+i\bar{h}_q^f$ (39). However, such an independent analysis becomes unimportant with realization of the SAMMY scheme, and in practice our problem reduces to finding the parameters of the combined method from the known parameters of the **R** or **K** matrix (3).

For this we use the RM approximation (12) and establish relations between the reduced matrices $\mathscr{R}_{nn}$, $\mathscr{R}_{fn}$, and $\mathscr{R}_{ff}$, where the subscript f refers to the channels remaining after radiative capture is excluded (in our case these are fission channels), and the corresponding blocks of the $\mathbf{R}'(E)$ matrix (13). We write the inverse level matrix $\mathbf{B}^{-1}$ (31) in this approximation as

$$\mathbf{B}^{-1}=\frac{1}{\mathscr{E}'-\mathbf{E}-\boldsymbol{\gamma}_f\bar{\mathbf{L}}_f\boldsymbol{\gamma}_f^{\mathrm{T}}}=\frac{1}{\mathscr{E}'-\mathbf{E}}\left[1+\boldsymbol{\gamma}_f\bar{\mathbf{L}}_f\boldsymbol{\gamma}_f^{\mathrm{T}}\frac{1}{\mathscr{E}'-\mathbf{E}-\boldsymbol{\gamma}_f\bar{\mathbf{L}}_f\boldsymbol{\gamma}_f^{\mathrm{T}}}\right], \tag{42}$$

where $\mathscr{E}'=\mathscr{E}-i\Gamma_\gamma/2$ is a diagonal matrix with elements $E'_\lambda=E_\lambda-i\Gamma_{\lambda\gamma}/2$, and $\boldsymbol{\gamma}_f$ is a rectangular ($\lambda\times f$) matrix with the number of columns equal to the number of fission channels. Multiplying both sides of this identity on the right and left by the corresponding matrices $\boldsymbol{\gamma}_n$ and $\boldsymbol{\gamma}_f$ ($\boldsymbol{\gamma}_n^{\mathrm{T}}$ and $\boldsymbol{\gamma}_f^{\mathrm{T}}$), we find

$$\mathscr{R}_{nn}=\mathbf{R}'_{nn}+\mathbf{R}'_{nf}\bar{\mathbf{L}}_f\mathscr{R}_{fn},\quad \mathscr{R}_{fn}=\mathbf{R}'_{fn}+\mathbf{R}'_{ff}\bar{\mathbf{L}}_f\mathscr{R}_{fn},$$
$$\mathscr{R}_{ff}=\mathbf{R}'_{ff}+\mathbf{R}'_{ff}\bar{\mathbf{L}}_f\mathscr{R}_{ff}\quad(\mathscr{R}_{ff}=(1-\mathbf{R}'_{ff}\bar{\mathbf{L}}_f)^{-1}\mathbf{R}'_{ff}). \tag{43}$$

These relations also follow from the equivalence of the two forms of the reduced $\mathscr{R}$ matrix (31) and (33).

As a specific example involving two fission channels $f=1,2$ realized in the SAMMY scheme, the matrix elements $\mathscr{R}_{ff}$ (for $\bar{L}_{1,2}=iP_{1,2}$) are written as

$$\mathscr{R}_{11}=\frac{1}{D}(R'_{11}-iP_2\rho_{12}),\quad \mathscr{R}_{22}=\frac{1}{D}(R'_{22}-iP_1\rho_{12}),$$
$$\mathscr{R}_{12}=\frac{1}{D}R'_{12}, \tag{44}$$

where

$$\rho_{12}=R'_{11}R'_{22}-(R'_{12})^2=\sum_{\lambda=1}^{N}\frac{\alpha_\lambda}{E'_\lambda-E},$$
$$\alpha_\lambda=\sum_{\mu\neq\lambda}^{N}\frac{(\gamma_{\lambda1}\gamma_{\mu2}-\gamma_{\lambda2}\gamma_{\mu1})^2}{E'_\mu-E'_\lambda},$$
$$D=|1-R'_{ff}\bar{L}_f|_2=1-\sum_{\lambda=1}^{N}\frac{a_\lambda}{E'_\lambda-E},$$
$$a_\lambda=iP_1\gamma_{\lambda_1}^2+iP_2\gamma_{\lambda2}^2+P_1P_2\alpha_\lambda, \tag{45}$$

and the elements of the $\mathbf{R}'$ matrix (13) are sums over an arbitrary but finite number of levels N (Appendix 3). Multiplying the numerator and denominator of the elements (44) by the product

$$\prod_{\lambda=1}^{N}(E'_\lambda-E),$$

we obtain ratios of polynomials in E. The further transformations are similar to those used in Sec. 2 for the AA method (the POLLA code[14]) and reduce to finding the N different roots of the polynomial in the denominator:

$$D(E)\prod_{\lambda=1}^{N}(E'_\lambda-E)=\prod_{q=1}^{N}(\bar{E}_q-E). \tag{46}$$

Representing the ratio of polynomials in the form of expansions in simple fractions (28),

$$\mathscr{R}_{11}=\sum_{q=1}^{N}\bar{\gamma}_{q1}^2/(\bar{E}_q-E),\quad \mathscr{R}_{22}=\sum_{q=1}^{N}\bar{\gamma}_{q2}^2/(\bar{E}_q-E),$$

$$\mathscr{R}_{12}=\sum_{q=1}^{N}\bar{\gamma}_{q1}\bar{\gamma}_{q2}/(\bar{E}_q-E),$$

we find the parameters

$$\bar{\gamma}_{q1}^2=\Theta_q[R'_{11}(\bar{E}_q)-iP_2\rho_{12}(\bar{E}_q)],$$

$$\bar{\gamma}_{q2}^2=\Theta_q[R'_{22}(\bar{E}_q)-iP_1\rho_{12}(\bar{E}_q)],$$

$$\bar{\gamma}_{q1}\bar{\gamma}_{q2}=\Theta_q R'_{12}(\bar{E}_q),$$

$$\Theta_q=\prod_{\lambda=1}^{N}(E'_\lambda-\bar{E}_q)\Big/\prod_{q'\neq q}^{N}(\bar{E}_{q'}-E_q). \tag{47}$$

This transformation is realized by the SIGMA program[16] and is formally equivalent to the scheme involving diagonalization of the matrix **B** by an orthogonal transformation.[12]

The parameters of the pole expansion for the elements $\mathscr{R}_{fn}$ of the matrix (43) are found in a similar manner:

$$\mathscr{R}_{1n}=\frac{1}{D}[R'_{1n}-iP_2(R'_{22}R'_{1n}-R'_{12}R'_{2n})]=\sum_{q=1}^{N}\frac{\bar{\gamma}_{q1}\bar{\gamma}_{qn}}{\bar{E}_q-E},$$

$$\mathscr{R}_{2n}=\frac{1}{D}[R'_{2n}-iP_1(R'_{11}R'_{2n}-R'_{21}R'_{1n})]=\sum_{q=1}^{N}\frac{\bar{\gamma}_{q2}\bar{\gamma}_{qn}}{\bar{E}_q-E}, \tag{48}$$

where

$$\bar{\gamma}_{q1}\bar{\gamma}_{qn}=\Theta_q\{R'_{1n}(\bar{E}_q)-iP_2[R'_{22}(\bar{E}_q)R'_{1n}(\bar{E}_q)-R'_{12}(\bar{E}_q)R'_{2n}(\bar{E}_q)]\}$$

$$\bar{\gamma}_{q2}\bar{\gamma}_{qn}=\Theta_q\{R'_{2n}(\bar{E}_q)-iP_1[R'_{11}(\bar{E}_q)R'_{2n}(\bar{E}_q)-R'_{21}(\bar{E}_q)R'_{1n}(\bar{E}_q)]\}. \tag{49}$$

Determining these products together with (47), we immediately find the parameters $\bar{\gamma}_{qn}^2$. We note that here the penetration factors of the fission channels P_1 and P_2 are independent of energy, but we use the above notation to indicate the generality of the conclusions. In practice they can be set equal to 1 by making the replacements $\sqrt{2}\bar{\gamma}_{q1,2}=\bar{\Gamma}_{q1,2}^{1/2}$ and $\sqrt{2}\gamma_{\lambda 1,2}=\Gamma_{\lambda 1,2}^{1/2}$.

In Table II we give the set of parameters of the combined method for ^{239}Pu:

$$\bar{E}_q=\bar{\mu}_q-i\bar{\nu}_q,\quad \bar{\Gamma}_{qn}^0=(2ka/\sqrt{E})\bar{\gamma}_{qn}^2,$$

$$\bar{G}_q^f=(2ka/\sqrt{E})\sum_{c(f)}\bar{g}_q^c$$

$$\left(\bar{H}_q^f=(2ka/\sqrt{E})\sum_{c(f)}\bar{h}_q^c\approx\mathrm{Im}\,\bar{\Gamma}_{qn}^0\right),$$

which lead to resonance cross sections identical to those from the SAMMY scheme (Fig. 1).

There are no fundamental difficulties in extending this scheme of transformation of the R-matrix parameters to the case of three or more fission channels if the corresponding data on the contribution of each channel are available. In addition, the inverse problem, i.e., transformation of the parameters of the combined method to the R-matrix parameters, appears fully capable of realization.

5. POLE EXPANSION OF THE *U* MATRIX

In contrast to the matrix representation of the energy dependence of the elements $U_{cn}(E)$ $[G_{cn}(E)]$ in the SAMMY scheme (2), the combined method defines mathematically identical functional relations for these elements in the form of ratios of sums of pole terms in E with the factors $L_n(E)$ explicitly isolated (35). However here, as before, the complicated energy dependence of the cross sections is preserved, and the Doppler broadening of the resonances, for example, can be included only by numerical integration. In addition, the rather simple expressions for the matrix elements G_{nn} and G_{an} (34) determined in the combined method explicitly illustrate the possibility of their further transformation to equivalent pole expansions.

Although, as already mentioned, the actual idea of the pole expansion of the collision matrix follows from the formalism of the Humblet–Rosenfeld theory of resonance reactions,[8] algorithms for the direct transformation of the R-matrix expressions for $\mathbf{U}(E)$ in (4) and (11) to identical pole forms have been found and programmed only recently by Hwang[17,18] (the WHOPPER code[17]).

Let us consider an example of such a transformation for the case of a single neutron channel and an arbitrary number of reaction channels, for which we assume $L_c=iP_c=\mathrm{const}$ $(c\neq n)$. In the combined method the elements of the collision matrix $U_{cn}(E)$ are defined as ratios of functions of energy (35). In particular, the diagonal element is

$$U_{nn}(E)=e^{-2i\varphi_n}[1-\mathscr{R}_{nn}(E)L_n(E)]^{-1}[1-\mathscr{R}_{nn}(E)L_n^*(E)], \tag{50}$$

where

$$\mathscr{R}_{nn}=\sum_{q=1}^{N}\bar{\gamma}_{qn}^2/(\bar{E}_q-E).$$

The logarithmic derivatives of neutron channels $L_n=L_l$ are functions of the variable $\rho=ka=\alpha E^{1/2}$ and can be written as ratios of known polynomials of degree l in k or $\sqrt{E}$ (Appendix 1):

$$\bar{L}_l(\sqrt{E})=i\alpha\sqrt{E}\bar{\Phi}_l(\sqrt{E})/\Phi_l(\sqrt{E}),$$

$$\bar{L}_l^*(\sqrt{E})=\bar{L}_l(-\sqrt{E}). \tag{51}$$

Similarly, the phase factor in (50) can be written as

$$e^{-2i\varphi_n}=e^{-2i\rho}\Phi_l(-\sqrt{E})/\Phi_l(\sqrt{E}). \tag{52}$$

We substitute these expressions into (50) and multiply the numerator and denominator by

$$\prod_{q=1}^{N}(E-\bar{E}_q).$$

Then U_{nn} takes the form of a ratio of polynomials of degree $2N+l$ in $\sqrt{E}$:

$$U_{nn}=e^{-2i\rho}Q^{(2N+l)}(-\sqrt{E})/Q^{(2N+l)}(\sqrt{E}), \tag{53}$$

where

$$Q^{(2N+l)}(\sqrt{E})=\alpha^{-l}\left[\Phi_l(\sqrt{E})\prod_{k=1}^{N}(E-\bar{E}_k)\right.$$

TABLE II. Parameters of the combined method for ^{239}Pu.

#	$\bar{\mu}_q$ [eV]	$\bar{\nu}_q$ [eV]	Re $\bar{\Gamma}^0_{qn}$ [eV$^{1/2}$]	Im $\bar{\Gamma}^0_{qn}$ [eV$^{1/2}$]	G^f_q [eV$^{1/2}$]	J
1	−1.5002E+2	1.1810E−1	3.5017E−2	1.7724E−5	2.8239E−2	1
2	−1.5467E+1	1.3426E−2	3.4454E−5	3.7983E−9	3.2718E−9	1
3	−6.7253E+0	6.8977E−1	4.7096E−3	3.0707E−5	3.8197E−3	0
4	−1.6705E−1	2.8381E−1	6.6072E−5	−1.6508E−6	6.6140E−5	0
5	2.9665E−1	4.8305E−2	1.4710E−4	−3.2058E−6	8.7230E−5	1
6	7.8170E+0	4.1188E−2	2.8289E−4	8.3775E−6	1.5322E−4	1
7	1.0931E+1	9.5041E−2	5.4277E−4	−4.0432E−5	4.3818E−4	1
8	1.1898E+1	2.9328E−2	2.8319E−4	2.8369E−5	9.7870E−5	1
9	1.4330E+1	4.4169E−2	1.5920E−4	3.5923E−5	1.0799E−4	1
10	1.4677E+1	3.4783E−2	4.9908E−4	−3.4116E−5	2.1878E−4	1
11	1.5481E+1	3.8772E−1	5.1584E−4	5.9756E−5	4.8787E−4	0
12	1.7657E+1	3.7323E−2	4.2908E−4	7.3761E−6	2.0912E−4	1
13	2.2266E+1	5.2288E−2	5.4865E−4	−1.1649E−5	3.3026E−4	1
14	2.3933E+1	3.0612E−2	1.7329E−5	3.7853E−6	7.0465E−6	1
15	2.6269E+1	4.0083E−2	3.0108E−4	6.5730E−6	1.5438E−4	1
16	2.7288E+1	2.0749E−2	2.8568E−5	−5.9072E−7	1.9461E−6	1
17	3.2341E+1	8.5920E−2	1.5299E−4	−1.0403E−5	1.1499E−4	0
18	3.5486E+1	2.2233E−2	4.5290E−5	9.3945E−8	3.6117E−6	1
19	4.1457E+1	2.7630E−2	5.1534E−4	−1.8391E−5	5.5075E−5	1
20	4.1736E+1	4.9397E−2	1.4254E−4	1.7746E−5	8.4850E−5	1
21	4.4531E+1	2.2201E−2	9.1891E−4	4.7583E−7	9.0465E−5	1
22	4.7657E+1	1.3654E−1	7.5621E−4	−4.5742E−5	6.6420E−4	0
23	4.9837E+1	3.7252E−1	5.7772E−4	2.1183E−5	5.4210E−4	0
24	5.0144E+1	1.3747E−2	4.5954E−4	−6.4607E−7	8.3470E−5	1
25	5.2648E+1	2.6489E−2	1.3041E−3	−1.0559E−5	2.2238E−4	1
26	5.5704E+1	3.0902E−2	2.0164E−4	9.5319E−6	7.8965E−5	1
27	5.7521E+1	4.8474E−1	2.9440E−3	−1.2090E−3	2.7907E−3	0
28	5.9292E+1	6.6270E−2	5.7717E−4	1.1906E−5	4.2957E−4	1
29	6.2810E+1	3.9221E+0	2.4702E−3	1.6033E−3	2.4498E−3	0
30	6.3171E+1	5.3839E−2	7.9248E−5	3.1718E−6	5.3465E−5	1
31	6.5343E+1	1.6554E−1	1.8308E−4	−2.8108E−4	1.5898E−4	0
32	6.5793E+1	8.5382E−2	1.1950E−3	−4.1060E−5	7.6350E−4	1
33	7.4168E+1	3.0427E−2	3.6807E−4	6.1105E−5	1.7860E−4	1
34	7.4940E+1	1.7167E−1	3.3310E−4	−8.2165E−5	2.9091E−4	0
35	7.5033E+1	6.4628E−2	2.4163E−3	−3.6803E−5	1.6664E−3	1
36	7.9085E+1	2.4000E−2	4.8085E−6	6.3463E−7	5.7680E−7	1
37	8.1183E+1	8.9264E−1	4.4572E−4	−9.0978E−4	4.1511E−4	0
38	8.2774E+1	2.6000E−2	3.6395E−5	9.8468E−7	3.5931E−6	1
39	8.5531E+1	9.9764E−1	5.3377E−3	8.8836E−4	5.1770E−3	0
40	8.5618E+1	1.6023E−2	8.8554E−4	2.2929E−6	1.6208E−4	1
41	9.0850E+1	2.0675E−2	1.2811E−3	−2.2217E−6	2.2797E−4	1
42	9.3079E+1	2.0269E−2	6.9940E−5	1.0630E−6	4.9900E−6	1
	.....	.....	.....	.....	.....	.
	.....	.....	.....	.....	.....	.
400	9.9424E+2	3.7805E−2	5.9838E−4	−3.9601E−5	2.5650E−4	1
401	9.9797E+2	1.5213E−1	1.1571E−3	2.1899E−4	1.0418E−3	1
402	9.9866E+2	3.9174E−2	1.0874E−3	−1.4656E−4	5.3470E−4	1
403	1.0050E+3	2.3595E−2	2.4363E−3	2.6225E−6	6.1425E−5	1
404	1.0093E+3	2.2617E+0	5.8504E−3	5.0642E−5	5.7900E−3	0
405	1.1000E+3	4.3992E−2	3.6784E−2	−2.6026E−5	1.7553E−2	1

$$+i\alpha\sqrt{E}\bar{\Phi}_l(\sqrt{E})\sum_{k=1}^{N}\bar{\gamma}^2_{kn}\prod_{k'\neq k}^{N}(E-\bar{E}_{k'})\Bigg].$$

Now, finding the $2N+l$ roots of this polynomial $\tilde{E}_k^{1/2}$ and assuming that they are nondegenerate, we represent the ratio in (53) as an expansion in simple fractions:

$$U_{nn}=e^{-2i(\rho-\pi l/2)}\left(1+i\sum_{k=1}^{2N+l}\frac{r_{kn}}{\tilde{E}_k^{1/2}-E^{1/2}}\right), \qquad (54)$$

where

$$r_{kn}=i\prod_{k'=1}^{2N+l}(\tilde{E}_k^{1/2}+\tilde{E}_k^{1/2})\Big/\prod_{k'\neq k}^{2N+l}(\tilde{E}_k^{1/2}-\tilde{E}_{k'}^{1/2})$$

are complex constants.

We isolate from the sum over k in (54) the N_1 terms ($1\leqslant k\leqslant N_1$) with $\mathrm{Re}\tilde{E}_k^{1/2}>0$ associated with the resonances observed in the energy range of interest and transform U_{nn} to the form

$$U_{nn}(E)=e^{-2i(\rho-\pi l/2)}\left(W^0_{nn}(E)+2i\sqrt{E}\sum_{k=1}^{N_1}\frac{r_{kn}}{\tilde{E}_k-E}\right), \tag{55}$$

where

$$W^0_{nn}(E)=1+i\sum_{k=N_1+1}^{2N+l}\frac{r_{kn}}{\tilde{E}_k^{1/2}-E^{1/2}}+i\sum_{k=1}^{N_1}\frac{r_{kn}}{\tilde{E}_k^{1/2}+E^{1/2}} \tag{56}$$

does not have poles in the range in question, thereby forming a smooth, energy-dependent background. As a result, we arrive at the representation of **U** as a sum of resonance and nonresonance components commonly used in the theory of nuclear reactions. It is similar in form to the corresponding result of the Kapur–Peierls formalism (17) with energy-independent parameters $\tilde{E}_k=\mu_k-i\nu_k$ and $\tilde{\gamma}^2_{kn}$, but with obligatory (even in the one-level case) isolation of the background part (56) correlated with the parameters of the N_1 resonances. Using $U_{nn}(E)$ (55) in the definition of the total cross section (1), we obtain the same multilevel expression (18) as in the AA method with the potential cross section

$$\sigma_p(E)=2\pi k^{-2}\sum_J g(J)[1-\mathrm{Re}\,e^{-2i(\rho-\pi l/2)}W^{0J}_{nn}(E)]. \tag{57}$$

It is also straightforward to construct the pole form for the absorption cross section $\sigma_a(E)$ (1) summed over all reaction channels. For this we again return to the expansion of $U_{nn}(E)$ (55) and write

$$1-|U_{nn}|^2=2\,\mathrm{Re}(-i)\sum_{k=1}^{2N+l}\frac{r_{ka}}{\tilde{E}_k^{1/2}-E^{1/2}}, \tag{58}$$

where

$$r_{ka}=r_{kn}\left(1-i\sum_{k'=1}^{2N+l}\frac{r^*_{k'n}}{\tilde{E}_k^{1/2*}-\tilde{E}_k^{1/2}}\right)$$

are also quantities independent of energy. We then isolate the N_1 (or N_{1J} for each independent system J) resonance terms from the sum over k in (58) and form from them a sum with poles in the physical E region similar to (55), including the other terms in the nonresonance background. In the end we again arrive at the result of the AA method (18), but with isolated and formally defined background absorption cross section:

$$\sigma_a(E)=\sigma^0_a(E)+4\pi k^{-2}\sqrt{E}\sum_J g(J)\times\sum_{k=1}^{N_{1J}}\mathrm{Re}(-i)\frac{r_{ka}}{\tilde{E}_k-E}, \tag{59}$$

where

$$\sigma^0_a(E)=2\pi k^{-2}\sum_J g(J)\mathrm{Re}\left[(-i)\left(\sum_{k=N_{1J}+1}^{2N_J+l}\frac{r_{ka}}{\tilde{E}_k^{1/2}-E^{1/2}}+\sum_{k=1}^{N_{1J}}\frac{r_{ka}}{\tilde{E}_k^{1/2}+E^{1/2}}\right)\right].$$

A similar representation as a sum of resonance terms and a background part is obviously also possible for the cross sections in the individual reaction channels $c\neq n$. This follows, for example, from the pole expansion (34):

$$\begin{aligned}G_{cn}P_n^{1/2}&=\mathscr{R}_{cn}(1-\mathscr{R}_{nn}\bar{L}_n)^{-1}P_n^{1/2}\\&=(\alpha\sqrt{E})^{l+1/2}(\Phi_l/\Phi_l^*)^{1/2}\mathscr{R}_{cn}[\Phi_l(\sqrt{E})\\&\quad-i\alpha\sqrt{E}\,\bar{\Phi}_l(\sqrt{E})\mathscr{R}_{nn}]^{-1},\end{aligned} \tag{60}$$

where the penetration factor $P_n=P_l$ is chosen as (Appendix 1)

$$P_l(\sqrt{E})=(\alpha\sqrt{E})^{2l+1}/\Phi_l(\sqrt{E})\Phi_l^*(\sqrt{E})$$

and $L_n=L_l(\sqrt{E})$ (51). The expansion scheme is analogous to that used earlier with transformation to a ratio of polynomials in $\sqrt{E}$ followed by expansion in partial fractions:

$$\begin{aligned}G_{cn}P_n^{1/2}&=(\alpha\sqrt{E})^{1/2}(\Phi_l/\Phi_l^*)^{1/2}\left[E^{l/2}\mathscr{R}_{cn}\prod_{q=1}^{N}(E-\bar{E}_q)/Q^{(2N+l)}(\sqrt{E})\right]\\&=(\alpha\sqrt{E})^{1/2}(\Phi_l/\Phi_l^*)^{1/2}\sum_{k=1}^{2N+l}\frac{\tilde{r}_{kc}}{\tilde{E}_k^{1/2}-E^{1/2}}\end{aligned} \tag{61}$$

with

$$\tilde{r}_{kc}=\tilde{E}_k^{l/2}\sum_{q=1}^{N}\bar{\gamma}_{qc}\bar{\gamma}_{qn}\prod_{q'\neq q}^{N}(\tilde{E}_k-\bar{E}_{q'})\Big/\prod_{k'\neq k}^{2N+l}(\tilde{E}_k^{1/2}-\tilde{E}_k^{1/2}).$$

The cross section for the (n,c) reaction for an individual system J is determined by the squared modulus of (61) and can be reduced to the form

$$\sigma^J_c(E)=4\pi k^{-2}g(J)P_c|G_{cn}P_n^{1/2}|^2=2\pi k^{-2}g(J)\times\mathrm{Re}(-i)\sum_{k=1}^{2N+l}\frac{r_{kc}}{\tilde{E}_k^{1/2}-E^{1/2}}, \tag{62}$$

where

$$r_{kc}=4i\tilde{r}_{kc}\alpha\tilde{E}_k^{1/2}\sum_{k'=1}^{2N+l}\frac{\tilde{r}^*_{k'c}}{\tilde{E}_k^{1/2*}-\tilde{E}_k^{1/2}}P_c.$$

The further transformations with isolation of the N_{1J} resonance terms in the sum (62) and formation of the background cross section are similar to the examples considered above in (57) and (61), and in the end lead to an expression for the cross section $\sigma_c(E)$ of the same form as (59) (with the subscript a replaced by c).

Thus, the rigorous pole expansion of the elements of the **U** matrix in the variable k (or $\sqrt{E}$) leads to formulas of the AA method giving the simplest representation of the energy dependence of the resonance cross sections as a sum of one-level terms and nonresonance background. However, the correct choice of parameters of the AA method and of the background part of the cross sections leading to results equivalent to those of the SAMMY scheme is established here by the

corresponding transformation of the R-matrix parameters or of the parameters of the combined method. Unfortunately, the inverse transformation, from the pole representation to the R-matrix parameters, is very problematical in general, because the pole parameters outside the range of resonance energies are mainly determined by the background part of the cross sections, which does not give much information for a unique determination of these parameters. Therefore, the results of model estimates of the contribution of nonresonance processes at relatively low energies can prove useful here.[2,3]

A more general version of the transformation of the collision matrix (11) to the pole form in $\sqrt{E}$, taking into account several neutron channels, is realized by the multipurpose WHOPPER code.[17] Here, as in the POLLA method,[15] the pole expansion is constructed directly for the elements of the matrix $\mathbf{A}^{-1}$ (26), where

$$A_{\lambda\mu}=(E_\lambda-E)\delta_{\lambda\mu}-i\Gamma^a_{\lambda\mu}/2-\sum_n \gamma_{\lambda n}L_n(\sqrt{E})\gamma_{\mu n} \quad (63)$$

with $\Gamma^a_{\lambda\mu}=\Gamma_{\lambda\gamma}\delta_{\lambda\mu}+\Gamma^f_{\lambda\mu}$ and $L_n=L_{l(n)}(\sqrt{E})$ (51). The solutions of the determinant equation $|\mathbf{A}(\sqrt{E})|_N=0$ determine the poles $\tilde{E}_k^{1/2}$, the number of which is $2N+\Sigma l$, where N is the rank of the matrix $\mathbf{A}$ (Appendix 3). The corresponding representation of $\mathbf{A}^{-1}$ is similar to (26):

$$(\mathbf{A}^{-1})_{\lambda\mu}=\frac{M_{\lambda\mu}(\sqrt{E})}{D(\sqrt{E})}=\sum_{k=1}^{2N+\Sigma l}\frac{m_{\lambda\mu}(\tilde{E}_k^{1/2})}{\tilde{E}_k^{1/2}-E^{1/2}}, \quad (64)$$

where

$$m_{\lambda\mu}(\tilde{E}_k^{1/2})=(-1)^{N+1}M_{\lambda\mu}(\tilde{E}_k^{1/2})\prod_l \Phi_l(\tilde{E}_k^{1/2})\alpha^l \Big/ \prod_{k'\neq k}^{2N+\Sigma l}(\tilde{E}_k^{1/2}-\tilde{E}_{k'}^{1/2}).$$

Substituting (64) into (11), we obtain a rigorous pole expansion for the elements of the $\mathbf{U}$ matrix:

$$U_{cn}=e^{-i\varphi_c}\left[\delta_{cn}+iP_c^{1/2}P_n^{1/2}\sum_{k=1}^{2N+\Sigma l}\beta_k^{cn}/(\tilde{E}_k^{1/2}-E^{1/2})\right]e^{-i\varphi_n}, \quad (65)$$

where

$$\beta_k^{cn}=2\sum_{\lambda\mu}\gamma_{\lambda c}\gamma_{\mu n}m_{\lambda\mu}(\tilde{E}_k^{1/2})$$

are complex constants. The rest of the procedure of isolating the N_1 resonance terms and the background component is similar to that considered above in (57) and (61) with, in general, the addition of the cross sections for elastic scattering between different neutron channels.

6. RESONANCE CROSS SECTIONS FOR INELASTIC SCATTERING

The mathematically identical methods of parametrizing resonance cross sections that we have considered here, the R-matrix method, the combined method, and the method with rigorous pole expansion of the $\mathbf{U}$ matrix (the Hwang method), are realized in practice at energies below the threshold for neutron inelastic scattering. This is completely sufficient for ground-state fissile nuclei. However, for many nonfissile isotopes resonance structure of the cross sections is also observed above threshold, both in the total cross sections and in the cross sections for excitation of the first level.[5,7,11]

For nonfissile nuclei the R-matrix approach in the RM approximation is equivalent to the combined method with reduced matrix $\mathbf{R}(E)$ (13). Formally, the inclusion of inelastic scattering reduces to the corresponding increase of the number of neutron channels n [the rank of the matrix $\mathbf{G}_{nn}$ (34)] and to the choice of the logarithmic derivatives of the inelastic channels (51) at energies $E-E_{\text{th}}$, where E_{th} is the threshold energy.

In the simplest example with one elastic scattering channel (n) and one inelastic scattering channel (n'), the elements of the $\mathbf{G}_{nn}$ matrix (34) are transformed as in (44) to the functional form characteristic of the combined method, i.e., a ratio of sums:

$$G_{nn}(E)=\sum_{\lambda=1}^{N}\frac{\gamma^2_{\lambda n}-\bar{L}_n\alpha_\lambda}{E'_\lambda-E}\Big/\left[1-\sum_{\lambda=1}^{N}\frac{a_\lambda}{E'_\lambda-E}\right],$$

$$G_{n'n}(E)=\sum_{\lambda=1}^{N}\frac{\gamma_{\lambda n'}\gamma_{\lambda n}}{E'_\lambda-E}\Big/\left[1-\sum_{\lambda=1}^{N}\frac{a_\lambda}{E'_\lambda-E}\right], \quad (66)$$

where

$$\alpha_\lambda=\sum_{\mu\neq\lambda}^{N}(\gamma_{\lambda n}\gamma_{\mu n'}-\gamma_{\mu n}\gamma_{\lambda n'})^2/(E'_\mu-E'_\lambda),$$

$$a_\lambda=\gamma^2_{\lambda n}\bar{L}_n+\gamma^2_{\lambda n'}\bar{L}_{n'}-\bar{L}_n\bar{L}_{n'}\alpha_\lambda.$$

Accordingly, the expressions for the cross sections determined by these elements are similar to those given in Sec. 3. However, here the singularities in the energy dependence determined by the function $L_n(E-E_{\text{th}})$ are taken into account near threshold not only for $E>E_{\text{th}}$, but also for negative $E-E_{\text{th}}$ (the closed-channel effect[1,2] in the total cross section and in the cross section for radiative capture).

The combined method, which in the RM approximation is equivalent to the corresponding SAMMY version,[7] fully reflects these features, and without difficulty can be extended to the case of several elastic and inelastic neutron channels. But the transformation of (66) to pole form is, in general, a more complicated problem than in the case where there is only elastic scattering (Sec. 5). In principle, here the elements of the $\mathbf{U}$ matrix are functions of two variables: the initial and final neutron energies. However, if we restrict ourselves to energies below, for example, the second level of the target nucleus (taking into account only the first level effective for a system with definite total angular momentum and parity), it is possible to construct a realizable algorithm for transforming the results of the combined method (66) to the equivalent pole forms only in the single variable $\sqrt{E}$.

In fact, the problem of the pole expansion here reduces mainly to representing G_{nn} and $G_{n'n}$ as ratios of polynomials. In our case, multiplying the numerator and denominator of (66) by the factor

$$\Phi_l(\rho)\Phi_{l'}(\rho')\prod_{\lambda=1}^{N}(E'_\lambda - E),$$

we represent the denominator of the ratio as

$$F_1(\sqrt{E}) - \sqrt{E-E_{\text{th}}}F_2(\sqrt{E}),$$

where $F_1(\sqrt{E})$ and $F_2(\sqrt{E})$ are polynomials in $\sqrt{E}$ (we shall not calculate their explicit expressions here). Multiplying both parts of the ratio by

$$F_1(\sqrt{E}) + \sqrt{E-E_{\text{th}}}F_2(\sqrt{E}),$$

we write the denominator as a polynomial in $\sqrt{E}$ of the form

$$F_1^2(\sqrt{E}) - (E-E_{\text{th}})F_2^2(\sqrt{E})$$

of degree $2(2N+l+l')$. The roots of this polynomial $\tilde{E}_k^{1/2}$ determine the complete set of poles in the corresponding pole expansion (66):

$$G_{n'n} = \sum_{k=1}^{2(2N+l+l')} \frac{d_k^{n'n}\sqrt{E} + f_k^{n'n}\sqrt{E-E_{\text{th}}}}{\tilde{E}_k^{1/2} - E^{1/2}}, \qquad (67)$$

where $d_k^{n'n}$, $f_k^{n'n}$, d_k^{nn}, and f_k^{nn} are complex constants determined by the R-matrix parameters according to schemes similar to those studied above in Sec. 5.

However, in applications where a parametric representation of the resonance cross sections is used over a wide energy range, it is apparently possible to restrict oneself to an approximate version of the pole expansion, where the level matrix (9) does not include the energy dependence of the logarithmic derivatives of the inelastic channels:[4]

$$\gamma_{\lambda n'}\bar{L}_{n'}(E)\gamma_{\mu n'} \approx \gamma_{\lambda n'}\bar{L}_{n'}^{1/2}(E_\lambda)\bar{L}_n^{1/2}(E_\mu)\gamma_{\mu n'}.$$

Then the pole expansion of the elements of the matrix $\mathbf{A}^{-1}$ is mathematically identical to the scheme studied above for fissile nuclei (Sec. 5) and can be realized for an arbitrary number of neutron channels, for example, by the WHOPPER code (63)–(65) (Ref. 17). The collision matrix is transformed to the form (65), where the features of the energy dependence above the inelastic-scattering threshold are taken into account by the corresponding penetration factors $P_n(E-E_{\text{th}})$ in the numerator of $U_{n'n}$ (65). Although such an approximation is no longer formally equivalent to the R-matrix parametrization (66), in practice it does not lead to any noticeable difference in the resonance cross sections or to paradoxical negative values, as in the AA method. In special cases where, for example, the shape of a resonance located right at the energy threshold is analyzed, it is possible to use the approximation of weak energy dependence in a restricted range of the logarithmic derivatives for elastic-scattering channels and to include this dependence exactly in inelastic channels. Then the level matrix $\mathbf{A}$ (9) is determined for the energy $E-E_{\text{th}}$, and the pole expansions of the elements of $\mathbf{A}^{-1}$ are constructed in terms of the variable $\sqrt{E-E_{\text{th}}}$.

CONCLUSION

We have seen that the advances in resonance-neutron spectrometry and the practical realization of the R-matrix SAMMY scheme in the multilevel analysis and estimation of the resonance cross sections has led to a significant increase in the amount of data on the resonance parameters.[5–7] The RM approximation used in this scheme along with neglect of the energy dependence of the level-shift parameter are valid for most nuclei. Of course, doubts remain about the uniqueness of determining the sets of parameters of the $\mathbf{R}$ (or $\mathbf{K}$) matrix, and the appearance of new data may lead to changes, for example, inclusion of the third fission channel of ^{235}U in the analysis. The statistical analysis of the distributions of R-matrix parameters does not reveal noticeable differences from the known regularities, but intermediate structures are manifested more clearly in the new data (Fig. 1). The interference of these structures with compound resonances is very interesting from the viewpoint of analyzing the spread of the intermediate states and checking the corresponding sum rules.[1–3,9]

The transformation of the R-matrix parameters to the parameters of other formalisms or of practical methods of multilevel representation of cross sections (the combined method and the Hwang method) has in the end proved to be a problem which can be solved on a PC, using modern programs for the inversion of complex matrices of large rank. The combined method is noteworthy for being closest in structure to the R-matrix parametrization. Independent determination of the parameters of the combined method for fissile nuclei may give information about the uniqueness of the choice of the corresponding R-matrix parameters, and for nonfissile nuclei it may allow estimation of the error from neglecting the level-shift factor in the SAMMY code, especially in the energy range where values $l \geqslant 1$ are effective and near the inelastic-scattering threshold. Moreover, the functional form of the energy dependence of $\mathbf{U}(E)$ (35) is preferable to the R-matrix form (2) for the statistical theory of cross sections averaged over resonances.[1–4]

Finally, the transformation to the rigorous pole expansion of the $\mathbf{U}$-matrix elements in the momentum variable $(\sqrt{E})$ serves as both the methodological foundation of the AA method and a practical recipe for constructing the corresponding level parameters and determining the background part of the cross sections. Here the representation of the cross sections as sums of one-level terms makes it elementary to include the temperature broadening of resonances by replacing the Breit–Wigner form of their energy dependence by the known Doppler functions Ψ and X (of the Voight profile; Refs. 5 and 17). Using it, many of the standard methods of the one-level approximation—averaging the cross sections over resonances, analysis of the neutron transmission functions for beams broad in energy, and calculations of the self-screening factors of resonances in problems of neutron transport in media—can be brought to the multilevel representation without significant changes.[3]

This review has focused mainly on the problems of judiciously choosing methods for estimating and representing the large amount of data presently available on the resonance

structure of neutron cross sections, using sets of energy-independent parameters. The use of these methods in modern libraries of nuclear data undoubtedly represents a qualitative advance in providing information for applied problems. In addition, the huge increase in the volume of data on neutron resonances also provides rich material both for refining the methods of the theory of resonance reactions, and for physical representations of the nuclear reaction mechanism and the structure of states of a compound nucleus.

It is possible to give several examples of the efficiency of the multilevel representation of the cross sections from the R-matrix analysis of light nuclei[11] up to resonance parametrization at high energies.[19] Results interesting for the physics of fission have been obtained in a multilevel interpretation of the data on the angular distributions of fission fragments for aligned nuclei.[20] The great increase in the amount of data on neutron resonances will certainly, sooner or later, attract the attention of theoreticians and perhaps provide a stimulus for new physical ideas.

APPENDIX 1. LOGARITHMIC DERIVATIVES AND PHASE SHIFTS FOR NEUTRON CHANNELS

Here we give the basic relations for the logarithmic derivatives of the exterior solutions L_c and for the phase shifts φ_c in the collision matrix $\mathbf{U}(E)$ (4). According to the general definition,[3-5]

$$L_c=\left[x_c O_l^{-1}(x_c)\frac{d}{dx_c}O_l(x_c)\right]_{x_c=\rho_c}=S_c(\rho_c)+iP_c(\rho_c), \tag{1.1}$$

$$e^{-2i\varphi_c}=I_l(\rho_c)/O_l(\rho_c),\quad \rho_c=k_c a_c, \tag{1.2}$$

where $O_l(x_c)$ and $I_l(x_c)=O_l^*(x_c)$ are functions of the parameter $x_c=k_c r_c$. They are the radial solutions of the scattering problem in the exterior region $r_c\geqslant a_c$, where there is no nuclear interaction. The Wronskian of this pair of solutions is

$$I_l(x_c)O_l'(x_c)-O_l(x_c)I_l'(x_c)=2i, \tag{1.3}$$

and, accordingly, for the real and imaginary parts of L_c (1.1) we have

$$S_c(\rho_c)=\frac{1}{2}\rho_c\left[\frac{d}{dx_c}\left|O_1(x_c)\right|^2\right]_{x_c=\rho_c}/|O_1(\rho_c)|^2,$$

$$P_c(\rho_c)=\rho_c/|O_l(\rho_c)|^2. \tag{1.4}$$

The values of $S_c(\rho_c)$ determine the level-shift factors (9), and $P_c(\rho_c)$ are the penetration factors of the channel c. The definition of $\mathbf{U}(E)$ (4) involves the logarithmic derivatives

$$\bar{L}_c=L_c-b_c, \tag{1.5}$$

which differ from L_c in general by the arbitrary real constant of the boundary condition, b_c (Ref. 3).

For neutron channels with positive energy the solutions $O_l(x)$ $(x=x_n)$ are linear combinations of spherical Bessel functions[3] and can be written as

$$O_l(x)=-x[n_l(x)-ij_l(x)]=e^{i(x-\pi l/2)}x^{-l}\Phi_l(x), \tag{1.6}$$

where

$$\Phi_0=1,\quad \Phi_1(x)=x+i,\quad \Phi_2(x)=x^2+3ix-3,$$

$$\Phi_l(x)=x^2\Phi_{l-2}(x)+i(2l-1)\Phi_{l-1}(x), \tag{1.7}$$

which follows from the recursion relations

$$O_l(x)=(l/x)O_{l-1}(x)-O_{l-1}'(x),\quad O_0(x)=e^{ix},$$

$$lO_l(x)+xO_l'(x)=xO_{l-1}(x)\quad (l\geqslant 1). \tag{1.8}$$

The last relation also determines the logarithmic derivatives of the neutron channels $L_l(\rho)$ (1.1) for $x=\rho=k_n a_n=\alpha\sqrt{E}=0.22\times 10^{-3}a_n\sqrt{E\,(\text{eV})}$ (a_n is the nuclear radius in units of 10^{-13} cm):

$$l+L_l(\rho)=i\rho\frac{\bar{\Phi}_l(\rho)}{\Phi_l(\rho)}=\frac{i\rho\bar{\Phi}_l(\rho)\Phi_l^*(\rho)}{\Phi_l(\rho)\Phi_l^*(\rho)}=i\rho\left[1+i\sum_{k=1}^{l}\frac{1}{\rho_k^{(l)}-\rho}\right], \tag{1.9}$$

where $\bar{\Phi}_l(\rho)=\rho\Phi_{l-1}(\rho)$, and $\rho_k^{(l)}$ are the roots of the polynomial $\Phi_l(\rho)$ (1.7). The different forms of the representation of $L_l(\rho)$ here illustrate the structure of the dependence of the logarithmic derivative on ρ as a ratio of polynomials or an expansion in simple poles. It is also obvious that the choice of boundary-condition constants $b_l=-l$ is convenient for neutron channels, so that

$$\bar{L}_l(\rho)=L_l(\rho)+l=\bar{S}_l(\rho)+iP_l(\rho), \tag{1.10}$$

and for $l=0,1,2$ we have

$$\bar{L}_0(\rho)=i\rho,\quad \bar{L}_1(\rho)=i\rho\frac{\rho}{\rho+i}=\frac{\rho^2+i\rho^3}{1+\rho^2}=i\rho\left[1+i\frac{1}{-i-\rho}\right],$$

$$\bar{L}_2(\rho)=i\rho\frac{\rho(\rho+i)}{\rho^2+3i\rho-3}=\frac{\rho^2(3+2\rho^2+i\rho^3)}{9+3\rho^2+\rho^4}$$

$$=i\rho\left[1+i\sum_{k=1}^{2}\frac{1}{\rho_k^{(2)}-\rho}\right]\left(\rho_{1,2}^{(2)}=-\frac{3}{2}i\pm\frac{\sqrt{3}}{2}\right). \tag{1.11}$$

The real and imaginary parts of $\bar{L}_l(\rho)$ (1.10) are expressed in terms of the functions $\Phi_l(\rho)$ as (1.4):

$$\bar{S}_l(\rho)=S_l(\rho)+l=\frac{1}{2}\rho\frac{[\Phi_l(\rho)\Phi_l^*(\rho)]}{\Phi_l(\rho)\Phi_l^*(\rho)},$$

$$P_l(\rho)=\frac{\rho^{2l+1}}{\Phi_l(\rho)\Phi_l^*(\rho)}. \tag{1.12}$$

The neutron phase shifts $\varphi_l(\rho)$ (1.2) can also be written as

$$e^{-2i\varphi_l}=(-1)^l e^{-2i\rho}\Phi_l^*(\rho)/\Phi_l(\rho), \tag{1.13}$$

or

$$\tan(\varphi_l-\rho-\pi l/2)=\text{Im}\,\Phi_l(\rho)/\text{Re}\,\Phi_l(\rho),$$

which leads to the well known expressions for the phase shifts:[3]

$$\varphi_0=\rho,\quad \varphi_1=\rho-\tan^{-1}\rho,\quad \varphi_2=\rho-\tan^{-1}\frac{3\rho}{3-\rho^2}. \tag{1.14}$$

The logarithmic derivatives of the neutron channels are analytic functions of $\rho(\sqrt{E})$, which we use in the pole expansion of $\mathbf{U}(E)$ (5). As the analytic continuation to negative energies, we can also use the logarithmic derivatives of closed neutron channels,

$$L_l^-(|\rho|)=L_l(i\rho)=S_l^-(|\rho|), \quad P_l^-(|\rho|)=0, \tag{1.15}$$

which are needed, in particular, for analyzing the energy dependence near the inelastic-scattering threshold E_{th}, where $\rho=\alpha\sqrt{E-E_{\text{th}}}$ (Refs. 1 and 2).

APPENDIX 2. UNITARITY RELATIONS

The basic expression for the collision matrix in R-matrix theory (4) is unitary and symmetric for arbitrary values of the real parameters. If we use the alternative representation in terms of the level matrix (10), the unitarity condition $\mathbf{UU}^+=1$ corresponds to a relation for the matrix $\mathbf{G}$ (7):

$$\mathbf{G}-\mathbf{G}^*=2i\mathbf{GPG}^* \tag{2.1}$$

or, using the definition (8), the matrix identity

$$\mathbf{A}^*-\mathbf{A}=2i\boldsymbol{\gamma}\mathbf{P}\boldsymbol{\gamma}^{\mathrm{T}}, \quad A^*_{\lambda\mu}-A_{\lambda\mu}=2i\sum_c \gamma_{\lambda c}P_c\gamma_{\mu c}, \tag{2.2}$$

corresponding to the definition of the level matrix $\mathbf{A}$ (9).

Going to the Kapur–Peierls formalism amounts to diagonalizing the level matrix $\mathbf{A}$ by an orthogonal transformation (16):

$$\tilde{\boldsymbol{\varepsilon}}-\mathbf{E}=\mathbf{VAV}^{\mathrm{T}} \quad (\mathbf{VV}^{\mathrm{T}}=1).$$

We write the identity (2.2) as

$$\mathbf{VA}^*\mathbf{V}^+-\mathbf{VAV}^+=2i\mathbf{V}\boldsymbol{\gamma}\mathbf{P}\boldsymbol{\gamma}^{\mathrm{T}}\mathbf{V}^+ \quad [\mathbf{V}^+=(\mathbf{V}^{\mathrm{T}})^*], \tag{2.3}$$

or

$$(\mathbf{VV}^+)\tilde{\boldsymbol{\varepsilon}}^*-\tilde{\boldsymbol{\varepsilon}}(\mathbf{VV}^+)=2i\tilde{\boldsymbol{\gamma}}\mathbf{P}\tilde{\boldsymbol{\gamma}}^+, \quad \tilde{\boldsymbol{\gamma}}=\mathbf{V}\boldsymbol{\gamma}.$$

Then,

$$(\mathbf{VV}^+)_{kk'}=2i\sum_c (\tilde{\gamma}_{kc}P_c\tilde{\gamma}^*_{k'c})/(\tilde{E}^*_{k'}-\tilde{E}_k), \tag{2.4}$$

and, multiplying both sides of this expression by $\tilde{\gamma}^*_{k'n}$ and summing over k', we obtain relations between the parameters of the formalism:

$$\tilde{\gamma}_{kn}=2i\sum_c\sum_{k'} (\tilde{\gamma}^*_{k'n}\tilde{\gamma}_{kc}\tilde{\gamma}^*_{k'c}P_c)/(\tilde{E}^*_{k'}-\tilde{E}_k), \tag{2.5}$$

corresponding to unitarity of the matrix $\mathbf{U}$ (17). Introducing the combinations of parameters used in the expressions for the cross sections (3),

$$g^c_k+ih^c_k=2i\sum_{k'} (\tilde{\gamma}_{kn}\tilde{\gamma}_{kc}\tilde{\gamma}^*_{k'n}\tilde{\gamma}^*_{k'c}P_c)/(\tilde{E}^*_{k'}-\tilde{E}_k), \tag{2.6}$$

we can also write the unitarity relation (2.5) as

$$\tilde{\gamma}^2_{kn}=\sum_c (g^c_k+ih^c_k). \tag{2.7}$$

In general, it is possible for energy dependence to arise here via the penetration factors $P_c(E)$. These are relations between complex constants only in the Adler approximation, where in Eqs. (2.4)–(2.6) it is assumed that $P_c(E)\approx$ const. Elimination of the radiative capture channels greatly decreases the number of parameters in (2.5) and, for example, in the special case of identical radiative widths of the levels, $\Gamma_{\lambda\gamma}=\Gamma_\gamma$, we have

$$\tilde{\gamma}_{kn}=2i\sum_{c\neq c(\gamma)}\sum_{k'} (\tilde{\gamma}^*_{k'n}\tilde{\gamma}_{kc}\tilde{\gamma}^*_{k'c}P_c)/(\tilde{E}^*_{k'}-\tilde{E}_k-i\Gamma_\gamma). \tag{2.8}$$

The combined method (Sec. 3) uses the block representation of the matrix $\mathbf{G}$, and in this case the unitarity relation (2.1) can be written, for example, as

$$\mathbf{G}_{nn}-\mathbf{G}^*_{nn}=2i[\mathbf{G}_{nn}\mathbf{P}_n\mathbf{G}^*_{nn}+\mathbf{G}_{na}\mathbf{P}_a\mathbf{G}^*_{an}]. \tag{2.9}$$

Substituting $\mathbf{G}_{nn}$ and $\mathbf{G}_{an}$ (34), we obtain the corresponding relation between the reduced R matrices:

$$\mathscr{R}_{nn}-\mathscr{R}^*_{nn}=2i\mathscr{R}_{na}\mathbf{P}_a\mathscr{R}^*_{an}$$

$$\left(\operatorname{Im}\mathscr{R}_{nn}=\sum_{c\neq n}P_c\left|\mathscr{R}_{cn}\right|^2\right). \tag{2.10}$$

If the R-matrix form (31) is used for the elements of these matrices, we will have an identity similar to (2.2) for the level matrix $\mathbf{B}$ (32):

$$B^*_{\lambda\mu}-B_{\lambda\mu}=2i\sum_{c\neq n}\gamma_{\lambda c}P_c\gamma_{\mu c}, \tag{2.11}$$

and for $\mathscr{R}_{cn}$ with diagonal level matrix (33) we find, using a scheme like that considered for the Kapur–Peierls formalism, the relation between the parameters of the combined method:

$$\bar{\gamma}_{qn}=2i\sum_{q'}\bar{\gamma}^*_{q'n}\sum_{c\neq n}(\bar{\gamma}_{qc}P_c\bar{\gamma}^*_{q'c})/(\bar{E}^*_{q'}-\bar{E}_q). \tag{2.12}$$

If both sides of (2.12) are multiplied by γ_{qn} and the parameters $\bar{g}^c_q+i\bar{h}^c_q$ (37) are introduced, we arrive at the relation

$$\bar{\gamma}^2_{qn}=\sum_{c\neq n}(\bar{g}^c_q+i\bar{h}^c_q). \tag{2.13}$$

Although outwardly these results are similar to those obtained above for the Kapur–Peierls formalism (2.6)–(2.8), here there are no terms containing neutron channels $P_n(E)$. Therefore, with the general assumption of weak energy dependence of the penetration factors for the reaction channels P_c $(c\neq n)$, the unitarity relations of the combined method (2.12) and (2.13) are sum rules for the complex, energy-independent parameters of the method.

APPENDIX 3. DETERMINANTS OF THE MATRICES $(1-\mathbf{R}\bar{\mathbf{L}})$

For two channels 1 and 2, this determinant can fairly easily be brought to the form

$$|1-\mathbf{R}\bar{\mathbf{L}}|_2=1-R_{11}\bar{L}_1-R_{22}\bar{L}_2+(R_{11}R_{22}-R_{12}R_{21})\bar{L}_1\bar{L}_2$$

$$=1-\sum_{\lambda=1}^{N}\frac{a^{(2)}_\lambda}{E_\lambda-E}, \tag{3.1}$$

where

$$a_\lambda^{(2)}=\lambda_{\lambda 1}^2\bar{L}_1+\lambda_{\lambda 2}^2\bar{L}_2-\bar{L}_1\bar{L}_2\sum_{\mu\neq\lambda}^{N}\frac{(\gamma_{\lambda 1}\gamma_{\mu 2}-\gamma_{\lambda 2}\gamma_{\mu 1})^2}{E_\mu-E_\lambda}, \tag{3.2}$$

and the elements of the R matrix (5) [or the $\mathscr{R}$ matrix (33)] are sums over a finite number of levels N.

In the case of three channels we write the determinant as a sum:

$$|1-\mathbf{R}\bar{\mathbf{L}}|_3=1-\sum_{i=1}^{3}R_{ii}\bar{L}_i+\sum_{i=1}^{3}\sum_{k>i}^{3}\bar{L}_i\bar{L}_k\begin{vmatrix}R_{ii}R_{ik}\\R_{ki}R_{kk}\end{vmatrix}-\bar{L}_1\bar{L}_2\bar{L}_3\begin{vmatrix}R_{11}R_{12}R_{13}\\R_{21}R_{22}R_{23}\\R_{31}R_{32}R_{33}\end{vmatrix}, \tag{3.3}$$

where the last determinant can be written as

$$|\mathbf{R}|_3=\begin{vmatrix}R_{11}R_{12}R_{13}\\R_{21}R_{22}R_{23}\\R_{31}R_{32}R_{33}\end{vmatrix}=\sum_{\lambda=1}^{N}\sum_{\mu\neq\lambda}^{N}\sum_{\nu\neq\mu}^{N}\frac{\gamma_{\lambda 1}\gamma_{\mu 2}\gamma_{\nu 3}}{(E_\lambda-E)(E_\mu-E)(E_\nu-E)}\begin{vmatrix}\gamma_{\lambda 1}\gamma_{\lambda 2}\gamma_{\lambda 3}\\\gamma_{\mu 1}\gamma_{\mu 2}\gamma_{\mu 3}\\\gamma_{\nu 1}\gamma_{\nu 2}\gamma_{\nu 3}\end{vmatrix} \tag{3.4}$$

with summation over the level indices λ, $\mu\neq\lambda$, and $\nu\neq\mu$. Subsequent expansion in simple fractions gives six products of the form

$$\frac{1}{E_\lambda-E}\frac{1}{E_\mu-E_\lambda}\frac{1}{E_\nu-E_\mu},$$

differing by permutations of the indices λ, μ, and ν. However, under these permutations only the sign of the determinant on the right-hand side of (3.4) changes, which ultimately leads to the pole expansion:

$$|\mathbf{R}|_3=\sum_{\lambda}^{N}\frac{1}{E_\lambda-E}\sum_{\mu\neq\lambda}^{N}\sum_{\nu\neq\mu}^{N}\frac{1}{(E_\mu-E_\lambda)(E_\nu-E_\mu)}\times\begin{vmatrix}\gamma_{\lambda 1}\gamma_{\lambda 2}\gamma_{\lambda 3}\\\gamma_{\mu 1}\gamma_{\mu 2}\gamma_{\mu 3}\\\gamma_{\nu 1}\gamma_{\nu 2}\gamma_{\nu 3}\end{vmatrix}^2. \tag{3.5}$$

As a result, for the third-order determinant we obtain a representation similar to (3.1):

$$|\mathbf{1}-\mathbf{RL}|_3=1-\sum_{\lambda=1}^{N}\frac{a_\lambda^{(3)}}{E_\lambda-E},$$

$$a_\lambda^{(3)}=\sum_{i=1}^{3}\gamma_{\lambda 1}^2\bar{L}_i-\sum_{\mu\neq\lambda}^{N}\frac{1}{E_\mu-E_\lambda}\sum_{i=1}^{3}\sum_{k>i}^{3}\bar{L}_i\bar{L}_k\begin{vmatrix}\gamma_{\lambda i}\gamma_{\lambda k}\\\gamma_{\mu i}\gamma_{\mu k}\end{vmatrix}^2+\sum_{\mu\neq\lambda}^{N}\sum_{\nu\neq\mu}^{N}\frac{\bar{L}_1\bar{L}_2\bar{L}_3}{(E_\mu-E_\lambda)(E_\nu-E_\mu)}\begin{vmatrix}\gamma_{\lambda 1}\gamma_{\lambda 2}\gamma_{\lambda 3}\\\gamma_{\mu 1}\gamma_{\mu 2}\gamma_{\mu 3}\\\gamma_{\nu 1}\gamma_{\nu 2}\gamma_{\nu 3}\end{vmatrix}^2 \tag{3.6}$$

The corresponding transformation of the nth-order determinant uses the well known expansion in the principal minors of the matrix $\mathbf{Q}=\mathbf{R}\bar{\mathbf{L}}$ (Ref. 21):

$$|1-\mathbf{Q}|_n=1-\sum_{i=1}^{n}Q_{ii}+\sum_{i=1}^{n}\sum_{k>i}^{n}\begin{vmatrix}Q_{ii}Q_{ik}\\Q_{ki}Q_{kk}\end{vmatrix}+\ldots+(-1)^n\begin{vmatrix}Q_{11}Q_{12}\cdots Q_{1n}\\\cdots\cdots\cdots\cdots\\Q_{n1}Q_{n2}\cdots Q_{nn},\end{vmatrix}, \tag{3.7}$$

and the minors themselves represent the Gram determinant,[22] calculated in our case as

$$\begin{vmatrix}Q_{11}Q_{12}\cdots Q_{1m}\\\cdots\cdots\cdots\cdots\\Q_{m1}Q_{m2}\cdots Q_{mm}\end{vmatrix}=\frac{1}{m!}\sum_{\lambda=1}^{N}\sum_{\mu\neq\lambda}^{N}\cdots\sum_{\theta\neq\theta-1}^{N}\frac{1}{(E_\lambda-E)(E_\mu-E)\ldots(E_0-E)}\begin{vmatrix}\gamma_{\lambda 1}\gamma_{\lambda 2}\cdots\gamma_{\lambda m}\\\gamma_{\mu 1}\gamma_{\mu 2}\cdots\gamma_{\mu m}\\\cdots\cdots\cdots\cdots\\\gamma_{\theta 1}\gamma_{\theta 2}\cdots\gamma_{\theta m}\end{vmatrix}^2. \tag{3.8}$$

The expansion in simple fractions gives $m!$ products of the form

$$\frac{1}{E_\lambda-E}\frac{1}{E_\mu-E_\lambda}\frac{1}{E_\nu-E_\mu}\cdots\frac{1}{E_\theta-E_{\theta-1}}$$

with various permutations of the indices under which the square of the determinant $|\gamma|_m$ does not change. In the end we again arrive at the representation (3.1):

$$|\mathbf{1}-\mathbf{R}\bar{\mathbf{L}}|_n=1-\sum_{\lambda=1}^{N}\frac{a_\lambda^{(n)}}{E_\lambda-E}, \tag{3.9}$$

with

$$a_\lambda^{(n)}=\sum_{i=1}^{n}\gamma_{\lambda_i}^2\bar{L}_i-\sum_{\mu\neq\lambda}^{N}\frac{1}{E_\mu-E_\lambda}\sum_{i=1}^{n}\sum_{k>i}^{n}\bar{L}_i\bar{L}_k\begin{vmatrix}\gamma_{\lambda i}\gamma_{\lambda k}\\\gamma_{\mu i}\gamma_{\mu k}\end{vmatrix}^2+\sum_{\mu\neq\lambda}^{N}\sum_{\nu\neq\mu}^{N}\frac{1}{(E_\mu-E_\lambda)(E_\nu-E_\mu)}\times\sum_{i=1}^{n}\sum_{k>i}^{n}\sum_{j>i}^{n}\begin{vmatrix}\gamma_{\lambda_i}\gamma_{\lambda k}\gamma_{\lambda j}\\\gamma_{\mu i}\gamma_{\mu k}\gamma_{\nu j}\\\gamma_{\nu i}\gamma_{\nu k}\gamma_{\nu j}\end{vmatrix}^2\bar{L}_i\bar{L}_k\bar{L}_j+\ldots$$

$$+(-1)^{n-1}\sum_{\mu\neq\lambda}^{N}\sum_{\nu\neq\mu}^{N}\cdots\sum_{\theta\neq\theta-1}^{N}$$

$$\times\frac{\bar{L}_1\bar{L}_2\ldots\bar{L}_n}{(E_\mu-E_\lambda)(E_\nu-E_\mu)\ldots(E_\theta-E_{\theta-1})}$$

$$\times\left|\begin{array}{c}\gamma_{\lambda 1}\gamma_{\lambda 2}\cdots\gamma_{\lambda n}\\ \gamma_{\mu 1}\gamma_{\mu 2}\cdots\gamma_{\mu n}\\ \cdots\cdots\cdots\\ \gamma_{\theta 1}\gamma_{\theta 2}\cdots\gamma_{\theta n}\end{array}\right|^2, \qquad (3.10)$$

where the summation over $i,k,j,\ldots$ pertains to the various principal minors of the determinant $|\gamma|_n$ of the last term in (3.10).

In the same way, it can be shown that the determinant of the corresponding level matrix **A** (9) is

$$D(E)=|\mathbf{A}|=|\mathbf{1}-\mathbf{RL}|_n\prod_{\lambda=1}^{N}(E_\lambda-E)=\prod_{\lambda=1}^{N}(E_\lambda-E)$$

$$-\sum_{\lambda=1}^{N}a_\lambda^{(n)}\prod_{\mu\neq\lambda}^{N}(E_\mu-E). \qquad (3.11)$$

Here we give a simpler version of the proof, using the matrix relation (7) in the form

$$\mathbf{G\bar{L}}=\boldsymbol{\gamma}^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\gamma}\bar{\mathbf{L}}=(\mathbf{1}-\mathbf{R\bar{L}})^{-1}-\mathbf{1}.$$

From this equation, for the diagonal elements (nn) in particular we have

$$(\mathbf{G\bar{L}})_{nn}=\sum_{\lambda\mu}\gamma_{\lambda n}(\mathbf{A}^{-1})_{\lambda\mu}\gamma_{\mu n}\bar{L}_n=\sum_{\lambda\mu}\gamma_{\lambda n}\frac{M_{\lambda\mu}(E)}{D}\gamma_{\mu n}\bar{L}_n$$

$$=\frac{|\mathbf{1}-\mathbf{R\bar{L}}|_{n-1}}{|\mathbf{1}-\mathbf{R\bar{L}}|_n}-1=\sum_{\lambda=1}^{N}(a_\lambda^{(n)}-a_\lambda^{(n-1)})$$

$$\times\prod_{\mu\neq\lambda}^{N}(E_\mu-E)/\left[\prod_{\lambda=1}^{N}(E_\lambda-E)|\mathbf{1}-\mathbf{R\bar{L}}|_n\right], \qquad (3.12)$$

where $M_{\lambda\mu}(E)$ is the cofactor of the matrix **A** (26). Equation (3.11) obviously follows from equality of the denominators.

For the Adler method, where the energy dependence of the logarithmic derivatives is neglected, we thereby explicitly determine the characteristic polynomial of the level matrix **A**, the N roots of which, $\tilde{E}_k$, correspond to poles of the $\mathbf{U}(E)$ matrix (17). The roots of the determinant of the matrix **B** (32) in the combined method are found in exactly the same way, but excluding neutron channels. In going to the pole expansion of the collision matrix in the wave number k (or $\sqrt{E}$) (6), our functional representation of the determinant $D(\sqrt{E})$ (3.11) explicitly includes the dependence of the logarithmic derivatives of the channels on $\rho=ka$ (Appendix 1). At energies below the neutron inelastic-scattering threshold the number of roots of the equation $D(\sqrt{E})=0$ (3.11) is

$$2N+l_{n1}+l_{n2}+\ldots, \qquad (3.13)$$

where n_i are the various neutron elastic-scattering channels possible for fixed values of the total angular momentum and parity, which follows directly from the definition of the coefficients $a_\lambda^{(n)}$ (3.10) and the rational representation of $\bar{L}_l(\rho)$ (1.9).

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