A NOTE ON THE ADLER–ADLER RESONANCE FORMALISM

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Abstract

Over restricted energy ranges, the Adler–Adler method of parameterizing resonance cross sections is in general the exact result of inverting the channel matrix. This provides a simple analytical form for the cross section which can be used in reactor physics calculations.

I. Introduction

The standard theory of resonance absorption of neutrons in reactors (Dresner 1960) assumes explicitly that all resonant cross sections can be written as a simple sum of contributions from single level Breit–Wigner (1936) contours which are corrected analytically to allow for Doppler broadening. However, it was realized by Vogt (1958) and Reich and Moore (1958) that such a sum is a crude approximation to the exact result of inverting the level matrix (Lane and Thomas 1958) and becomes inadequate especially when resonances are close together as in fissile isotopes. Resonance–resonance interference terms were derived by the above authors which provided a much better fit to the cross sections of fissile elements but which contained more parameters than the sum of Breit–Wigner contours. Unfortunately, the multilevel formulae obtained were too complicated to allow for Doppler broadening analytically, or to be employed in reactor resonance absorption theory.

More recently, Adler and Adler (1963) used a perturbation expansion approximation to derive expressions for cross sections which have the appearance of a sum of single level contributions with a symmetric and antisymmetric term for each level. Such a form can be employed in reactor resonance theory using the methods of Cook and Kletzmayr (1967), and Doppler broadening can be allowed for analytically. It is the purpose of this paper to show that all multilevel theories can be reduced to the Adler–Adler form.

II. Inversion of the Level Matrix

In the standard R-matrix reaction theory (Lane and Thomas 1958) the cross section for a reaction from the incident channel c to the final channel c' is

$$\sigma_{cc'} = (\pi/k_c^2) \sum_{ljJj'l'} g_J \, | \, \delta_{clj,c'l'j'} - S_{clj,c'l'j'} \, |^2 , \tag{1}$$

where $S_{clj,c'l'j'}$ is the scattering matrix, $k_c^2 = 2\mu_c E_c$ with E_c and μ_c the energy and reduced mass in channel c respectively, l is the orbital angular momentum, j is the channel spin, J is the total angular momentum of the compound system, and

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$g_J = (2J+1)/2(2I+1)$, I being the spin of the target nucleus. If we neglect threshold reactions, E_c is independent of c and we can put $E_c = E$. The **S** matrix is related to the reaction matrix **R** by the equation for each (l,J) partial wave of

$$\mathbf{S} = \boldsymbol{\Omega}[\mathbf{I}+2\mathrm{i}\mathbf{P}^{\frac{1}{2}}(\mathbf{I}-\mathbf{R}\mathbf{L}_0)^{-1}\mathbf{R}\mathbf{P}^{\frac{1}{2}}]\boldsymbol{\Omega}\,, \tag{2}$$

where

$$R_{cc'} = \sum_{\lambda=1}^{n} \frac{f_{\lambda cc'}}{(E_\lambda - E)} + R^0_{cc'}\,, \qquad f_{\lambda cc'} = \gamma_{\lambda c}\gamma_{\lambda c'}\,, \tag{3a, b}$$

with n the number of levels considered, $R^0_{cc'}$ a background constant, the $\gamma_{\lambda c}$ real constants, and E_λ the energy at poles in **R**. In equation (2) $\boldsymbol{\Omega}$, **P**, and $\mathbf{L}_0$ are diagonal matrices with elements

$$\Omega_c = \exp(-\mathrm{i}\phi_c)\,,$$

ϕ_c being the hard sphere phase shift in channel c; P_c, which is the penetration factor; and

$$L_{0c} = S_c - B_c + \mathrm{i}P_c\,,$$

S_c being the level shift and the B_c constants arising from boundary conditions. In general, if the interaction potential is not a self-adjoint operator, the matrix $\mathbf{f}_\lambda$ is not of rank one.

Many authors have reported the evaluation of the above quantities (e.g. Preston 1962; Lynn 1968). We define the transition matrix **T** by

$$T_{cc'} = (S_{cc'} - \delta_{cc'})/2\mathrm{i}\,, \tag{4a}$$

giving

$$\mathbf{T} = (\boldsymbol{\Omega}^2 - \mathbf{I})/2\mathrm{i} + \boldsymbol{\Omega}\mathbf{P}^{\frac{1}{2}}(\mathbf{I}-\mathbf{R}\mathbf{L}_0)^{-1}\mathbf{R}\mathbf{P}^{\frac{1}{2}}\boldsymbol{\Omega}\,. \tag{4b}$$

The difficulties in finding a suitable parameterization for the **S** matrix arise from the fact that we ordinarily deal with reactions where there are at least 100 channels, and the inversion of the channel matrix $(\mathbf{I}-\mathbf{R}\mathbf{L}_0)$ is correspondingly difficult.

We begin this analysis by noting that equation (3a) can be expressed by grouping all terms as a ratio of polynomials in E:

$$R_{cc'} = N^{(n)}_{cc'}(E)/D^{(n)}(E)\,, \tag{5}$$

where

$$D^{(n)}(E) = \prod_{\lambda=1}^{n} (E_\lambda - E)$$

and $N^{(n)}_{cc'}(E)$ is a matrix of polynomials of order n. The quantity L_{0c} is usually considered to be a set of constants except in the scattering channel where it is a slowly varying function of E. However, since only algebraic operations are used in the following arguments, no error is introduced into the proof by regarding all of the L_{0c}'s as constants.

The matrix to be inverted is

$$W_{cc'} = \delta_{cc'} - N^{(n)}_{cc'}\,L_{0c'}/D^{(n)}(E) = G^{(n)}_{cc'}(E)/D^{(n)}(E)\,, \tag{6}$$

where $G_{cc'}^{(n)}(E)$ is a matrix of polynomials of order n. Therefore

$$[W^{-1}]_{cc'} = D^{(n)}(E)\,[G_{cc'}^{(n)}(E)]^{-1} = M_{cc'}^{(n(N-1))}(E)\,D^{(n)}(E)/\Delta^{(nN)}(E)\,, \tag{7}$$

where N is the number of channels c, $M_{cc'}^{(n(N-1))}(E)$ is the matrix of cofactors of $G_{cc'}^{(n)}(E)$ transposed, and is a polynomial of order $n(N-1)$ in E, and $\Delta^{(nN)}(E)$ is the determinant of $G_{cc'}^{(n)}(E)$ and is a polynomial of order nN in E.

Referring to equation (4b) we see that

$$\sum_{c'} P_c^{\frac{1}{2}}[W^{-1}]_{cc'}\,R_{c'c''}\,P_{c''}^{\frac{1}{2}} = \mathscr{P}_{cc''}^{(nN)}(E)/\Delta^{(nN)}(E)\,, \tag{8a}$$

where

$$\mathscr{P}_{cc''}^{(nN)} = \sum_{c'} P_c^{\frac{1}{2}}\,M_{cc'}^{(n(N-1))}(E)\,N_{c'c''}^{(n)}(E)\,P_{c''}^{\frac{1}{2}}\,, \tag{8b}$$

which is a polynomial of order nN in E. Therefore

$$S_{cc'} = \exp(\mathrm{i}\phi_c)\{\delta_{cc'} + 2\mathrm{i}\mathscr{P}_{cc'}^{(nN)}(E)/\Delta^{(nN)}(E)\}\exp(\mathrm{i}\phi_{c'})\,. \tag{9}$$

The poles in the **S** matrix occur at the zeros in the determinant $\Delta^{(nN)}(E)$. In general, if the matrix $\mathbf{f}_\lambda$ of residues for a given λ is of rank N, there will be nN zeros of the determinant $\Delta^{(nN)}(E)$ and consequently nN poles of the **S** matrix. However, the matrix $\mathbf{f}_\lambda$, being of the form in equation (3b), is of rank one for a given level λ. This produces $n(N-1)$ common factors in the ratio in equation (9) which can be seen as follows. Lane and Thomas (1958) note that if the **R** matrix is written as

$$\mathbf{R} = \mathbf{R}' + \mathbf{R}_0 \tag{10}$$

then

$$(\mathbf{I}-\mathbf{R}\mathbf{L}_0)^{-1}\mathbf{R} = (\mathbf{I}-\mathbf{R}_0\mathbf{L}_0)^{-1}\mathbf{R}_0 + (\mathbf{I}-\mathbf{R}_0\mathbf{L}_0)^{-1}(\mathbf{I}-\mathbf{R}'\mathbf{L}')^{-1}\mathbf{R}'(\mathbf{I}-\mathbf{L}_0\mathbf{R}_0)^{-1}\,, \tag{11}$$

where $\mathbf{L}'$ is defined as

$$\mathbf{L}' = \mathbf{L}_0(\mathbf{I}-\mathbf{R}_0\mathbf{L}_0)^{-1}\,. \tag{12}$$

The standard procedure is then to assume an expansion

$$(\mathbf{I}-\mathbf{R}'\mathbf{L}')^{-1}_{cc'} = \delta_{cc'} + \sum_\lambda \sum_\mu \gamma_{\lambda c}\beta_{\mu c'}\,A_{\mu\nu}(E)\,, \tag{13}$$

where

$$\boldsymbol{\beta}_\mu = \mathbf{L}'\boldsymbol{\gamma}_\mu\,.$$

Here $\boldsymbol{\gamma}_\mu$ is the vector of constants $\gamma_{\mu c}$ and $A_{\mu\nu}(E)$ is the inverse of the level matrix

$$\mathbf{A} = (\mathbf{e}-\mathbf{E}-\boldsymbol{\xi})^{-1}\,, \tag{14a}$$

where

$$\xi_{\lambda\mu} = \sum_c \beta_{\lambda c}\gamma_{\mu c}\,, \qquad e_{\lambda\mu} = E_\lambda\,\delta_{\lambda\mu}\,, \qquad E_{\lambda\mu} = E\delta_{\lambda\mu}\,. \tag{14b}$$

We then find that

$$(\mathbf{I}-\mathbf{R}'\mathbf{L}')^{-1}\mathbf{R}' = \sum_\lambda \sum_\mu \gamma_{\lambda c}\gamma_{\mu c'}\,A_{\lambda\mu}(E)\,. \tag{15}$$

The matrix $A_{\lambda\mu}$ can be expressed as

$$A_{\lambda\mu} = F^{(n-1)}_{\lambda\mu}(E)/\Delta^{(n)}(E) = \sum_{\rho=1}^{n} H^{\rho}_{\lambda\mu}/(E-Z_{\rho}), \tag{16}$$

where $F^{(n-1)}_{\lambda\mu}(E)$ is a polynomial of degree $n-1$ in E and $\Delta^{(n)}(E)$ is a polynomial of degree n in E, both with complex coefficients that may be slowly varying functions of E. The determinant $\Delta^{n}(E)$ has n zeros at complex values of $E = Z_{\rho}$ and equation (16) expresses the result of applying partial fractions to the ratio of polynomials. The $H^{\rho}_{\lambda\mu}$ are the complex residues of the poles in **A**. Therefore

$$((\mathbf{I}-\mathbf{R}'\mathbf{L}')^{-1}\mathbf{R}')_{cc'} = \sum_{\rho} B^{\rho}_{cc'}/(E-Z_{\rho}), \tag{17}$$

where

$$B^{\rho}_{cc'} = \sum_{\lambda}\sum_{\mu} H^{\rho}_{\lambda\mu}\gamma_{\lambda c}\gamma_{\mu c'}.$$

On substituting (17) into (11) and referring back to equation (4b), we get

$$T_{cc'} = T^{0}_{cc'} + U^{0}_{cc'} + U_{cc'}, \tag{18a}$$

where

$$T^{0}_{cc'} = [\exp\{\mathrm{i}(\phi_c+\phi_{c'})\}-1]\delta_{cc'}/2\mathrm{i}, \tag{18b}$$

$$U^{0}_{cc'} = \exp(\mathrm{i}\phi_c)\, P^{\frac{1}{2}}_{c}((\mathbf{I}-\mathbf{R}_0\mathbf{L}_0)^{-1}\mathbf{R}_0)_{cc'}\, P^{\frac{1}{2}}_{c'}\exp(\mathrm{i}\phi_{c'}), \tag{18c}$$

$$U_{cc'} = \exp(\mathrm{i}\phi_c)\, P^{\frac{1}{2}}_{c} K_{cc'}\, P^{\frac{1}{2}}_{c'}\exp(\mathrm{i}\phi_{c'}), \tag{18d}$$

and

$$\mathbf{K} = (\mathbf{I}-\mathbf{R}_0\mathbf{L}_0)^{-1}\sum_{\rho}\frac{\mathbf{B}^{\rho}}{E-Z_{\rho}}(\mathbf{I}-\mathbf{L}_0\mathbf{R}_0)^{-1} = \sum_{\rho}\frac{\mathbf{Q}^{\rho}}{E-Z_{\rho}}. \tag{18e}$$

This gives finally

$$T_{cc'} = T^{0}_{cc'} + U^{0}_{cc'} + \exp(\mathrm{i}\phi_c)\sum_{\rho=1}^{n}\frac{a^{\rho}_{cc'}}{E-Z_{\rho}}\exp(\mathrm{i}\phi_{c'}), \tag{19a}$$

with

$$a^{\rho}_{cc'} = P^{\frac{1}{2}}_{c} Q^{\rho}_{cc'} P^{\frac{1}{2}}_{c'}. \tag{19b}$$

There are therefore n complex poles of the **T** matrix, with complex residues $a^{\rho}_{cc'}$. In general it is not possible to write the residues in the form given by Moldauer (1964), namely

$$\exp\{\mathrm{i}(\phi_c+\phi_{c'})\}\, a^{\rho}_{cc'} = g_{\rho c}\, g_{\rho c'}, \tag{20}$$

so that the matrix $\mathbf{a}^{\rho}$ is not of rank one. However, Moldauer showed that if we make a Taylor series expansion of $a(E)$ in a sufficiently small interval around E_{ρ}, then the form of equation (20) is approximately correct. He also pointed out that the precise conditions which must be imposed on the interaction Hamiltonian in order to justify a Mittag–Leffler expansion of the multichannel collision matrix (equation (18e)) are not known. For fitting cross sections over restricted energy ranges, the energy dependences contained in $\mathbf{L}_0$ can be neglected, and the Humblet–Rosenfeld (1961) expansion is approximately valid.

III. Cross Sections

Writing the cross section in equation (1) as

$$\sigma_{cc'} = (4\pi/k_c^2)\,|\,T_{cc'}\,|^2 \tag{21}$$

and substituting equation (18a) into (21), we get

$$\sigma_{cc'} = (4\pi/k_c^2)[|\,T^0_{cc'}+U^0_{cc'}\,|^2+|\,U_{cc'}\,|^2+2\,\mathrm{Re}\{(T^0_{cc'}+U^0_{cc'})U^*_{cc'}\}]\,. \tag{22}$$

Let

$$Z_\rho = \mathscr{E}_\rho+\tfrac{1}{2}\mathrm{i}\Gamma_\rho\,, \tag{23a}$$

$$a^\rho_{cc'} = x^\rho_{cc'}+\mathrm{i}y^\rho_{cc'}\,, \tag{23b}$$

$$\exp\{-\mathrm{i}(\phi_c+\phi_{c'})\}(T^0_{cc'}+U^0_{cc'}) = C_{cc'}+\mathrm{i}D_{cc'}\,, \tag{23c}$$

where $\mathscr{E}_\rho$, Γ_ρ, $x^\rho_{cc'}$, $y^\rho_{cc'}$, $C_{cc'}$, and $D_{cc'}$ are real quantities. Substituting (19a) into (21) and using equations (23), we get for each $(jlJj'l')$

$$\sigma_{cc'} = \sigma^{\mathrm{b}}_{cc'}+\sigma^{\mathrm{s}}_{cc'}+\sigma^{\mathrm{a}}_{cc'}\,, \tag{24}$$

where, after some manipulation and applying the partial fraction device used by Cook and Kletzmayr (1967), we get

$$\sigma^{\mathrm{b}}_{cc'} = (4\pi/k_c^2)|\,T^0_{cc'}+U^0_{cc'}\,|^2\,, \tag{25}$$

$$\sigma^{\mathrm{s}}_{cc'} = (\pi/k_c^2)\sum_\rho (\Gamma^\rho_{cc'})^2/\{(E-\mathscr{E}_\rho)^2+\tfrac{1}{4}\Gamma_\rho^2\} \tag{26a}$$

with

$$\tfrac{1}{4}(\Gamma'^\rho_{cc'})^2 = |\,a^\rho_{cc'}\,|^2-\Gamma_\rho\sum_{\mu\neq\rho}\left(\frac{\tfrac{1}{2}(\Gamma_\mu+\Gamma_\rho)(x^\rho_{cc'}x^\mu_{cc'}+y^\rho_{cc'}y^\mu_{cc'})+(\mathscr{E}_\mu-\mathscr{E}_\rho)(x^\mu_{cc'}y^\rho_{cc'}-x^\rho_{cc'}y^\mu_{cc'})}{(\mathscr{E}_\mu-\mathscr{E}_\rho)^2+\tfrac{1}{2}(\Gamma_\mu+\Gamma_\rho)^2}\right)$$

$$+(C_{cc'}y^\rho_{cc'}-D_{cc'}x^\rho_{cc'})\Gamma_\rho\,, \tag{26b}$$

and

$$\sigma^{\mathrm{a}}_{cc'} = (4\pi/k_c^2)\sum_\rho \eta^\rho_{cc'}(E-\mathscr{E}_\rho)/\{(E-\mathscr{E}_\rho)^2+\tfrac{1}{4}\Gamma_\rho^2\} \tag{27a}$$

with

$$\eta^\rho_{cc'} = 2\sum_{\mu\neq\rho}\left(\frac{(x^\rho_{cc'}x^\mu_{cc'}+y^\rho_{cc'}y^\mu_{cc'})(\mathscr{E}_\mu-\mathscr{E}_\rho)-\tfrac{1}{2}(\Gamma_\mu+\Gamma_\rho)(x^\mu_{cc'}y^\rho_{cc'}-x^\rho_{cc'}y^\mu_{cc'})}{(\mathscr{E}_\mu-\mathscr{E}_\rho)^2+\tfrac{1}{4}\Gamma_\rho^2}\right)$$

$$+2(C_{cc'}x^\rho_{cc'}+D_{cc'}y^\rho_{cc'})\,. \tag{27b}$$

In equations (25)–(27) $\sigma^{\mathrm{b}}_{cc'}$ is a slowly varying background cross section, $\sigma^{\mathrm{s}}_{cc'}$ has the form of a sum over symmetric contributions from single levels, and $\sigma^{\mathrm{a}}_{cc'}$ is the sum over corresponding asymmetric terms from single levels.

The great advantage of equation (24) in reactor resonance theory is that, if we neglect the effect of the slow variation of energy in the parameters, the Doppler-broadened cross section can be written (Cook and Kletzmayr 1967)

$$\langle \sigma_{cc'} \rangle_T = \overset{\mathrm{b}}{\sigma}_{cc'} + \sum_\rho \overset{0\rho}{\sigma}_{cc'} \psi(\theta_\rho, X_\rho) + (8\pi/k_c^2) \sum_\rho (\eta^\rho_{cc'}/\Gamma_\rho)\, \phi(\theta_\rho, X_\rho), \tag{28}$$

where $\langle\ \rangle_T$ denotes the average over atomic speeds,

$$\theta_\rho = \frac{4E_\rho kT}{A\Gamma_\rho^2}, \qquad X_\rho = \frac{2(\mathscr{E}_\rho - E)}{\Gamma_\rho}, \qquad \overset{0\rho}{\sigma}_{cc'} = \frac{4\pi}{k_c^2}\left(\frac{\Gamma^\rho_{cc'}}{\Gamma_\rho}\right)^2,$$

$$\psi(\theta, X) = \frac{1}{2(\pi\theta)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \frac{\exp\{-(x-y)^2/4\theta\}\, \mathrm{d}y}{1+y^2},$$

$$\phi(\theta, X) = \frac{1}{2(\pi\theta)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \frac{\exp\{-(x-y)^2/4\theta\} y\, \mathrm{d}y}{1+y^2},$$

with A the atomic mass of the absorbing nucleus, k Boltzmann's constant, and T the temperature in kelvin.

This is the form of parameterization used by Adler and Adler (1963), and it follows from the above arguments that all multilevel schemes for inverting the channel matrix or level matrix must be transformable to the same parameterization. Of the available formalisms for dealing with fissile isotopes, this is by far the most elementary and therefore the most convenient means of fitting cross sections to obtain parameters for use in reactor physics calculations.

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V. References

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