

APPROVED FOR PUBLICATION

D. Lang
B55
AAEC/TM606

AAEC/TM606



28

**AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS**

A NOTE ON THE ADLER-ADLER RESONANCE FORMALISM

by

J.L. COOK

November 1971

APPROVED FOR PUBLICATION

ISBN 0 642 99441 2

AUSTRALIAN ATOMIC ENERGY COMMISSION

RESEARCH ESTABLISHMENT

LUCAS HEIGHTS

A NOTE ON THE ADLER-ADLER RESONANCE FORMALISM

by

J. L. COOK

ABSTRACT

Over restricted energy ranges, the Adler-Adler method of parameterising 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.

Note: This paper has been submitted to a journal. Further details can be obtained from the author or the Director of the Research Establishment.

National Library of Australia card number and ISBN 0 642 99441 2

The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA-INIS-12 (INIS: Manual for Indexing) and IAEA-INIS-13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency.

ANALYTICAL SOLUTION; COLLISION MATRIX; CROSS SECTIONS; DOPPLER EFFECT;
ENERGY LEVELS; NEUTRONS; RESONANCE ABSORPTION; S-MATRIX; SYMMETRY;
WIGNER-EISENBUD THEORY.

CONTENTS

	<u>Page</u>
1. INTRODUCTION	1
2. INVERSION OF THE LEVEL MATRIX	1
3. CROSS SECTIONS	6
4. CONCLUSION	9
5. ACKNOWLEDGEMENTS	9
6. REFERENCES	9

1. 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 realised 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 such 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 the 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 anti-symmetric term for each level. Such a form can be employed in reactor resonance theory using the methods of Cook and Kletzmayer (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.

2. 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

$$\sigma_{cc'} = \frac{\pi}{k_c^2} \sum_{l_j J_j l'_{j'}} g_J \left| \delta_{cl_j, c'l'_{j'}} - S_{cl_j, c'l'_{j'}} \right|^2 \quad \dots(1)$$

where

$S_{cl_j, c'l'_{j'}}$ = scattering matrix

k_c^2 = $2 \mu_c E_c$

E_c = the energy in channel c

μ_c = the reduced mass in channel c

l = orbital angular momentum

j = channel spin

I = spin of target nucleus

J = total angular momentum of the compound system

$$g_J = \frac{2J+1}{2(2I+1)} .$$

If we neglect threshold reactions, E_c is independent of c so we can put $E_c = E$. The \underline{S} matrix is related to the reaction matrix \underline{R} by the equation for each (l, J) partial wave of

$$\underline{S} = \underline{\Omega} \left[\underline{I} + 2i \underline{P}^{\frac{1}{2}} (\underline{I} - \underline{R} \underline{L}_0)^{-1} \underline{R} \underline{P}^{\frac{1}{2}} \right] \underline{\Omega} \quad \dots(2)$$

where

$$R_{cc'} = \sum_{\lambda=1}^n \frac{f_{\lambda cc'}}{E_{\lambda} - E} + R_{cc'}^0 \quad \dots(3)$$

$$f_{\lambda cc'} = \gamma_{\lambda c} \gamma_{\lambda c'} \quad \dots(4)$$

n = number of levels considered

$R_{cc'}^0$ = background constant

$\gamma_{\lambda c}$ = real constants

E_{λ} = energy at poles in \underline{R} .

$\underline{\Omega}$, \underline{P} , \underline{L}_0 are diagonal matrices with elements

$$\Omega_c = e^{-i\phi_c}$$

where ϕ_c = hard sphere phase shift in channel c ,

P_c = penetration factor,

and $L_c^0 = S_c - B_c + iP_c$

where S_c = level shift

B_c = constants arising from boundary conditions.

In general, if the interaction potential is not a self-adjoint operator, the matrix \underline{f}_{λ} is not of rank one.

Many authors have reported the evaluation of the above quantities, for example Preston (1962), Lynn (1968). We define the transition matrix \underline{T} by

$$T_{cc'} = \frac{1}{2i} (S_{cc'} - \delta_{cc'}) \quad \dots(5)$$

giving

$$\underline{T} = \frac{1}{2i} (\underline{\Omega}^2 - \underline{I}) + \underline{\Omega} \underline{P}^{\frac{1}{2}} (\underline{I} - \underline{R} \underline{L}^0)^{-1} \underline{R} \underline{P}^{\frac{1}{2}} \underline{\Omega} \quad \dots(5a)$$

The difficulties in finding a suitable parameterisation for the \underline{S} matrix arise from the fact that we ordinarily deal with reactions where there are at least a hundred channels, and the inversion of the channel matrix $(\underline{I} - \underline{R} \underline{L}^0)$ is correspondingly difficult.

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

$$R_{cc'} = \frac{N_{cc'}^{(n)}(E)}{D^{(n)}(E)} \quad \dots(6)$$

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

and $N_{cc'}^{(n)}(E)$ is a matrix of polynomials of order n .

The quantity L_c^0 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 we use only algebraic operations in the following arguments, no error is introduced into the proof by regarding all of the L_c^0 's as constants.

The matrix to be inverted is

$$W_{cc'} = \delta_{cc'} - \frac{N_{cc'}^{(n)} L_c^0}{D^{(n)}(E)} = \frac{G_{cc'}^{(n)}(E)}{D^{(n)}(E)} \quad \dots(7)$$

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

Therefore

$$\begin{aligned} [W^{-1}]_{cc'} &= D^{(n)}(E) [G_{cc'}^{(n)}(E)]^{-1} \\ &= M_{cc'}^{(n(N-1))}(E) \cdot D^{(n)}(E) / \Delta^{(nN)}(E) \end{aligned} \quad \dots(8)$$

where N = number of channels c ,

$M_{cc}^{(n(N-1))}(E)$ = the matrix of cofactors of $G_{cc}^{(n)}(E)$ transposed,
 = polynomial of order $n(N-1)$ in E ,

$\Delta^{(nN)}(E)$ = determinant of $G_{cc}^{(n)}(E)$
 = polynomial of order nN in E .

Referring to Equation (4) we see that

$$\sum_{c'} P_c^{\frac{1}{2}} [W^{-1}]_{cc'} R_{c'c''} P_{c''}^{\frac{1}{2}} = \frac{\mathcal{P}_{cc''}^{(nN)}(E)}{\Delta^{(nN)}(E)} \quad \dots(9)$$

$$\begin{aligned} \text{where } \mathcal{P}_{cc''}^{(nN)} &= \sum_{c'} P_c^{\frac{1}{2}} M_{cc'}^{(n(N-1))}(E) N_{c'c''}^{(n)}(E) P_{c''}^{\frac{1}{2}} \quad \dots(9a) \\ &= \text{polynomial of order } nN \text{ in } E. \end{aligned}$$

Therefore

$$S_{cc'} = e^{i\theta_c} \left[\delta_{cc'} + 2i \frac{\mathcal{P}_{cc'}^{(nN)}(E)}{\Delta^{(nN)}(E)} \right] e^{i\theta_{c'}} \quad \dots(10)$$

The poles in the \underline{S} matrix occur at the zeroes in the determinant $\Delta^{(nN)}(E)$. In general, if the matrix \underline{f}_λ of residues for a given λ is of rank N , there will be nN zeroes of the determinant $\Delta^{(nN)}(E)$ and consequently nN poles of the \underline{S} matrix. However, the matrix \underline{f}_λ , being of the form in Equation (4), is of rank one for a given level, λ . This produces $n(N-1)$ common factors in the ratio in Equation (10) which can be seen as follows. Lane and Thomas (1958) note that if the \underline{R} matrix is written as

$$\underline{R} = \underline{R}' + \underline{R}_0 \quad \dots(11)$$

then

$$(\underline{I} - \underline{R} \underline{L}_0)^{-1} \underline{R} = (\underline{I} - \underline{R}_0 \underline{L}_0)^{-1} \underline{R}_0 + (\underline{I} - \underline{R}_0 \underline{L}_0)^{-1} (\underline{I} - \underline{R}' \underline{L}')^{-1} \underline{R}' (\underline{I} - \underline{L}_0 \underline{R}_0)^{-1} \quad \dots(12)$$

where \underline{L}' is defined as

$$\underline{L}' = \underline{L}_0 (\underline{I} - \underline{R}_0 \underline{L}_0)^{-1} \quad \dots(13)$$

The standard procedure is then to assume an expansion

$$(\underline{I} - \underline{R}' \underline{L}')_{cc'}^{-1} = \delta_{cc'} + \sum_{\lambda} \sum_{\mu} \gamma_{\lambda c} \beta_{\mu c'} A_{\lambda\mu}(E) \quad \dots(14)$$

where

$$\beta_{\mu} = \underline{L}' \chi_{\mu} .$$

χ_{μ} is the vector of constants $\gamma_{\mu c}$,

and $A_{\lambda\mu}(E)$ is the inverse of the level matrix

$$\underline{A} = (\underline{e} - \underline{E} - \underline{\xi})^{-1} \quad \dots(15)$$

where

$$\xi_{\lambda\mu} = \sum_c \beta_{\lambda c} \gamma_{\mu c} \quad \dots(15a)$$

$$e_{\lambda\mu} = E_{\lambda} \delta_{\lambda\mu} \quad \dots(15b)$$

$$E_{\lambda\mu} = E \delta_{\lambda\mu} . \quad \dots(15c)$$

We then find that

$$(\underline{I} - \underline{R}' \underline{L}')^{-1} \underline{R}' = \sum_{\lambda} \sum_{\mu} \gamma_{\lambda c} \gamma_{\mu c'} A_{\lambda\mu}(E) . \quad \dots(16)$$

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

$$A_{\lambda\mu} = \frac{F_{\lambda\mu}^{(n-1)}(E)}{\Delta^{(n)}(E)} = \sum_{\rho=1}^n \frac{H_{\lambda\mu}^{\rho}}{E - Z_{\rho}} \quad \dots(17)$$

where $F_{\lambda\mu}^{(n-1)}(E)$ 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 . $\Delta^{(n)}(E)$ has n zeroes at complex values of $E = Z_{\rho}$ and Equation (17) expresses the result of applying partial fractions to the ratio of polynomials. $H_{\lambda\mu}^{\rho}$ are the complex residues of the poles in \underline{A} . Therefore

$$[(\underline{I} - \underline{R}' \underline{L}')^{-1} \underline{R}']_{cc'} = \sum_{\rho} \frac{B_{cc'}^{\rho}}{E - Z_{\rho}} \quad \dots(18)$$

where $B_{cc'}^{\rho} = \sum_{\lambda} \sum_{\mu} H_{\lambda\mu}^{\rho} \gamma_{\lambda c} \gamma_{\mu c'} .$

On substituting (18) into (12) and referring back to Equation (5a), we get

$$T_{cc'} = T_{cc'}^0 + U_{cc'}^0 + U_{cc'} \quad \dots(19)$$

$$\text{with } T_{cc'}^0 = \frac{1}{2i} (e^{i(\vartheta_c + \vartheta_{c'})} - 1) \delta_{cc'} \quad \dots(19a)$$

$$U_{cc'}^0 = e^{i\vartheta_c} P_c^{\frac{1}{2}} [(\underline{I} - \underline{R_0 L_0})^{-1} \underline{R_0}]_{cc'} P_{c'}^{\frac{1}{2}} e^{i\vartheta_{c'}} \quad \dots(19b)$$

$$U_{cc'} = e^{i\vartheta_c} P_c^{\frac{1}{2}} K_{cc'} P_{c'}^{\frac{1}{2}} e^{i\vartheta_{c'}} \quad \dots(19c)$$

$$\text{and } \underline{K} = (\underline{I} - \underline{R_0 L_0})^{-1} \sum_{\rho} \frac{\underline{E}^{\rho}}{E - Z_{\rho}} (\underline{I} - \underline{L_0 R_0})^{-1} = \sum_{\rho} \frac{Q^{\rho}}{E - Z_{\rho}} \quad \dots(19d)$$

This gives finally

$$T_{cc'} = T_{cc'}^0 + U_{cc'}^0 + e^{i\vartheta_c} \sum_{\rho=1}^n \frac{a_{cc'}^{\rho}}{E - Z_{\rho}} e^{i\vartheta_{c'}} \quad \dots(20)$$

$$\text{with } a_{cc'}^{\rho} = P_c^{\frac{1}{2}} Q_{cc'}^{\rho} P_{c'}^{\frac{1}{2}} \quad \dots(20a)$$

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

$$\text{that is } e^{i(\vartheta_c + \vartheta_{c'})} a_{cc'}^{\rho} = g_{\rho c} g_{\rho c'} \quad \dots(21)$$

so that the matrix \underline{a}^{ρ} 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 (21) is approximately correct. Moldauer (1964) 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 (19d)) are not known. For fitting cross sections over restricted energy ranges, the energy dependences contained in \underline{L}^0 can be neglected, and the Humblet-Rosenfeld expansion (1961) is approximately valid.

3. CROSS SECTIONS

Writing the cross section in Equation (1) as

$$\sigma_{cc'} = \frac{4\pi}{k_c^2} \left| T_{cc'} \right|^2 \quad \dots(22)$$

and substituting Equation (19a) into (22), we get

$$\sigma_{cc'} = \frac{4\pi}{k_c^2} \left\{ |T_{cc'}^o + U_{cc'}^o|^2 + |U_{cc'}^o|^2 + 2 \operatorname{Re} (T_{cc'}^o + U_{cc'}^o) U_{cc'}^{*o} \right\} \quad \dots(23)$$

$$\text{Let } Z_\rho = \xi_\rho + i\Gamma_\rho/2 \quad \dots(24a)$$

$$a_{cc'}^\rho = x_{cc'}^\rho + iy_{cc'}^\rho \quad \dots(24b)$$

$$e^{-i(\theta_c + \theta_{c'})} (T_{cc'}^o + U_{cc'}^o) = C_{cc'} + iD_{cc'} \quad \dots(24c)$$

where ξ_ρ , Γ_ρ , $x_{cc'}^\rho$, $y_{cc'}^\rho$, $C_{cc'}$ and $D_{cc'}$ are real quantities.

Substituting (20) into (22) and using Equations (24) we get for each $(j \neq j' \neq l')$

$$\sigma_{cc'} = \sigma_{cc'}^b + \sigma_{cc'}^s + \sigma_{cc'}^a \quad \dots(25)$$

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

$$\sigma_{cc'}^b = \frac{4\pi}{k_c^2} |T_{cc'}^o + U_{cc'}^o|^2 \quad \dots(26)$$

$$\sigma_{cc'}^s = \frac{\pi}{k_c^2} \sum_\rho \frac{(\Gamma_{cc'}^\rho)^2}{(E - \xi_\rho)^2 + \Gamma_\rho^2/4} \quad \dots(27)$$

where

$$\begin{aligned} (\Gamma_{cc'}^\rho)^2/4 &= |a_{cc'}^\rho|^2 - \left\{ \Gamma_\rho \sum_{\mu \neq \rho} \frac{1}{2} (\Gamma_\mu + \Gamma_\rho) (x_{cc'}^\rho x_{cc'}^\mu + y_{cc'}^\rho y_{cc'}^\mu) + \right. \\ &+ (\xi_\mu - \xi_\rho) (x_{cc'}^\mu y_{cc'}^\rho - x_{cc'}^\rho y_{cc'}^\mu) \left. \right\} / ((\xi_\mu - \xi_\rho)^2 + \frac{1}{2} (\Gamma_\mu + \Gamma_\rho)^2) + \\ &+ (C_{cc'} y_{cc'}^\rho - D_{cc'} x_{cc'}^\rho) \Gamma_\rho \quad \dots(27a) \end{aligned}$$

$$\text{and } \sigma_{cc'}^a = \frac{4\pi}{k_c^2} \sum_\rho \frac{\eta_{cc'}^\rho (E - \xi_\rho)}{(E - \xi_\rho)^2 + \Gamma_\rho^2/4} \quad \dots(28)$$

$$\begin{aligned}
\text{where } \eta_{cc'}^{\rho} &= 2 \left\{ \sum_{\mu \neq \rho} \left[(x_{cc'}^{\rho}, x_{cc'}^{\mu} + y_{cc'}^{\rho}, y_{cc'}^{\mu}) (\xi_{\mu} - \xi_{\rho}) - \right. \right. \\
&- \left. \frac{1}{2} (\Gamma_{\mu} + \Gamma_{\rho}) (x_{cc'}^{\mu}, y_{cc'}^{\rho} - x_{cc'}^{\rho}, y_{cc'}^{\mu}) \right] / ((\xi_{\mu} - \xi_{\rho})^2 + \Gamma_{\rho}^2/4) \left. \right\} + \\
&+ 2 (C_{cc'}^{\rho}, x_{cc'}^{\rho} + D_{cc'}^{\rho}, y_{cc'}^{\rho}) \quad \dots(28a)
\end{aligned}$$

In Equations (26-28) $\sigma_{cc'}^b$ is a slowly-varying background cross section, $\sigma_{cc'}^s$ has the form of a sum over symmetric contributions from single levels, and $\sigma_{cc'}^a$ is the sum over corresponding asymmetric terms from single levels.

The great advantage of Equation (25) in reactor resonance theory is that if we neglect the effect of the slow energy-variation in the parameters, the Doppler-broadened cross section can be written (Cook and Kletzmayer 1967)

$$\begin{aligned}
\langle \sigma_{cc'} \rangle_T &= \sigma_{cc'}^b + \sum_{\rho} \sigma_{cc'}^{\text{op}} \cdot \psi(\theta_{\rho}, X_{\rho}) + \\
&+ \frac{8\pi}{k_c^2} \sum_{\rho} \left(\frac{\eta_{cc'}^{\rho}}{\Gamma_{\rho}} \right) \cdot \phi(\theta_{\rho}, X_{\rho}) \quad \dots(29)
\end{aligned}$$

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

$$\theta_{\rho} = 4 \frac{E k T}{A \Gamma_{\rho}^2}, \quad X_{\rho} = \frac{2}{\Gamma_{\rho}} (\xi_{\rho} - E), \quad \sigma_{cc'}^{\text{op}} = \frac{4\pi}{k_c^2} \left(\frac{\Gamma_{cc'}^{\rho}}{\Gamma_{\rho}} \right)^2,$$

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

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

where A = atomic mass of the absorbing nucleus,
 k = Boltzmann's constant
and T = temperature in degrees Kelvin.

This is the form of parameterisation 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 parameterisation. When dealing with fissile isotopes this is therefore the most convenient means of

fitting cross sections to obtain parameters for use in reactor physics calculations.

4. CONCLUSION

It was shown that all multilevel theories yield cross sections which are reducible to the Adler-Adler formalism and that this formalism, compared with others available, is by far the most elementary form to use when studying resonance absorption in reactors.

5. ACKNOWLEDGEMENTS

The author is grateful to Dr. W. K. Bertram for many enlightening discussions on reaction matrix theory.

6. REFERENCES

- Adler, D. B. and Adler, F. T. (1963). - ANL-6792.
- Breit, G. and Wigner, E. P. (1936). - Phys. Rev. 49, 519.
- Cook, J. L. and Kletzmayer, E. K. (1967). - Aust. J. Phys. 20, 253.
- Dresner, L. (1960). - 'Resonance Absorption in Nuclear Reactors' (Pergamon Press: London).
- Humblet, J. and Rosenfeld, L. (1961). - Nucl. Phys. 26, 529.
- Lane, A. M. and Thomas, R. G. (1958). - Rev. Mod. Phys. 30, 257.
- Lynn, J. E. (1968). - 'The Theory of Neutron Resonance Reactions' (Clarendon Press: Oxford).
- Moldauer, P. A. (1964). - Phys. Rev. 135, B642.
- Reich, C. W. and Moore, M. S. (1958). - Phys. Rev. 118, 718.
- Vogt, E. (1958). - Phys. Rev. 112, 203.
- Preston, M. A. (1962). - 'Physics of the Nucleus' (Addison-Wesley: Massachusetts).

