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A Note on Unitarity in Resonance Theory

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Abstract

Equations resulting from the unitarity of the collision matrix are investigated in standard resonance theory. The nonuniqueness or otherwise of fitted resonance parameters is discussed.

Introduction

In a recent paper, Adler and Adler (1972) showed that, given a set of cross sections for a fissile material, then in a perturbation approximation there is no unique solution for the reaction matrix parameters when there are more than two fission channels present. One difficulty in their approach is that their perturbative solutions do not satisfy unitarity, and it remains unclear as to whether their conclusions are general or depend upon the approximation used. In the present paper, the resonance theory is presented in a way slightly different from theirs, but one in which unitarity is easier to investigate. The conditions under which Kapur–Peierls (1938) reaction matrix parameters may be found are considered.

Background

Following Lane and Thomas (1958), the collision matrix elements can be written as

$$U_{cc'} = \exp\big(\mathrm{i}(\Omega_c+\Omega_{c'})\big)(\delta_{cc'}+\mathrm{i}T_{cc'}). \tag{1}$$

The transition matrix $T_{cc'}$ can be shown by standard theory to be given by

$$T_{cc'} = \sum_{\lambda\lambda'} A_{\lambda\lambda'}\gamma_{\lambda c}\gamma_{\lambda' c'}, \tag{2}$$

where γ_c is the reduced width of the reaction matrix, and **A** is the Wigner level matrix, defined as

$$A^{-1}_{\lambda\lambda'} = (E_\lambda - E)\delta_{\lambda\lambda'} - \mathrm{i}\Gamma_{\lambda\lambda'} \qquad \text{with} \qquad \Gamma_{\lambda\lambda'} = \tfrac{1}{2}\sum_c \gamma_{\lambda c}\gamma_{\lambda' c}, \tag{3,4}$$

while the reaction matrix **R** is given by

$$R_{cc'} = \sum_\lambda \gamma_{\lambda c}\gamma_{\lambda c'}/(E_\lambda - E). \tag{5}$$

The level matrix may be expressed in terms of its eigenvalues as

$$A_{\lambda\lambda'} = \sum_{\mu} S_{\lambda\mu} S_{\lambda'\mu}/(C_\mu - E), \qquad \text{where} \qquad C_\mu = \sum_{\lambda\lambda'} S_{\lambda\mu}(A^{-1}_{\lambda\lambda'} + \delta_{\lambda\lambda'} E) S_{\lambda'\mu} \tag{6,7}$$

are the complex eigenvalues of $\mathbf{A}^{-1} + \mathbf{I}E$, and $\mathbf{S}$ is a complex orthogonal matrix of the eigenvectors of $\mathbf{A}$. The $\mathbf{T}$ matrix (2) can then be written in the Kapur–Peierls (1938) form

$$T_{cc'} = \sum_{\mu} g_{\mu c} g_{\mu c'}/(C_\mu - E), \tag{8}$$

where the Kapur–Peierls reduced width is

$$g_{\mu c} = \sum_{\lambda} S_{\lambda\mu} \gamma_{\lambda c}. \tag{9}$$

The complex energy

$$C_\mu = \mu_\mu - \mathrm{i}\nu_\mu \tag{10}$$

can be interpreted as arising from a resonance at energy μ_μ with half-width ν_μ.

In the Adler–Adler theory, the cross sections

$$\sigma^{(x)}(E) = \sum_{c(x)} |U_{nc}|^2 \tag{11}$$

take the form

$$\sigma^{(x)}(E) = cE^{-\frac{1}{2}} \sum_{J} \sum_{\lambda} \{G^{(x)}_\lambda \nu_\lambda + (\mu_\lambda - E) H^{(x)}_\lambda\}/\{(\mu_\lambda - E)^2 + \nu^2_\lambda\} \tag{12}$$

for reaction cross sections and, for the total cross section, the form

$$\sigma^{\mathrm{T}}_n(E) = cE^{-\frac{1}{2}} \left\{ \sum_J \left(\sum_\lambda (\alpha^0_\lambda \cos\omega - \beta^0_\lambda \sin\omega)\nu_\lambda + \frac{(\mu_\lambda - E)(\alpha^0_\lambda \sin\omega + \beta^0_\lambda \cos\omega)}{(\mu_\lambda - E)^2 + \nu^2_\lambda} \right) + 2g_J E^{-\frac{1}{2}}(1 - \cos\omega) \right\}, \tag{13}$$

where c is a proportionality constant, ω is the potential scattering phase shift and g_J is the spin statistical weight factor, while λ is summed over states with the same J and parity. In this theory we have the important restriction

$$\alpha^0_\lambda + \mathrm{i}\beta^0_\lambda = g^2_{\lambda n} = \sum_{\mu\nu} S_{\mu\lambda} S_{\nu\lambda} \gamma_{\mu n} \gamma_{\nu n}. \tag{14}$$

The Adler–Adler coefficients, in terms of the Kapur–Peierls parameters, are

$$G^{(x)}_\lambda + \mathrm{i}H^{(x)}_\lambda = \sum_{\mu} X^{(n)}_{\lambda\mu} X^{(x)}_{\lambda\mu}/(C^*_\mu - C_\lambda), \qquad \text{where} \qquad X^{(x)}_{\lambda\mu} = \sum_{c(x)} g_{\lambda c} g^*_{\mu c}. \tag{15,16}$$

We can show also, from the orthogonality of $\mathbf{S}$ and the hermiticity of $\mathbf{X}$, that

$$\sum_\lambda \beta^0_\lambda = 0, \qquad \sum_\lambda H^{(x)}_\lambda = 0, \qquad \sum_x (G^{(x)}_\lambda + \mathrm{i}H^{(x)}_\lambda) = g^2_{\lambda n}. \tag{17a, b, c}$$

Adler–Adler Nonuniqueness

Adler and Adler (1972) showed that to first order in $\Gamma_{\lambda\lambda'}/(E_\lambda - E_{\lambda'})$ their parameters are given approximately by:

$$\alpha_\lambda^0 + \mathrm{i}\beta_\lambda^0 = \Gamma_{\lambda n}^0 + 2\mathrm{i} \sum_{\mu \neq \lambda} \Gamma_{\mu\lambda}\gamma_{\mu n}\gamma_{\lambda n}/(E_\mu - E_\lambda), \tag{18}$$

$$G_\lambda^{\mathrm{F}} + \mathrm{i}H_\lambda^{\mathrm{F}} = \Gamma_\lambda^0 \Gamma_{\lambda f}/2\Gamma_{\lambda\lambda} + 2\mathrm{i} \sum_{\mu \neq \lambda} \Gamma_{\mu\lambda}^0 \gamma_{\mu n}\gamma_{\lambda n}/(E_\mu - E_\lambda), \tag{19}$$

$$G_\lambda^\gamma = \Gamma_{\lambda n}^0 \Gamma_{\lambda\gamma}/2\Gamma_{\lambda\lambda} \quad \text{and} \quad H_\lambda^\gamma = 0, \tag{20a, b}$$

where

$$\Gamma_{\lambda\mu} = \Gamma_{\lambda\mu}^{\mathrm{F}} + \tfrac{1}{2}\gamma_{\mu n}\gamma_{\lambda n}, \quad \Gamma_{\lambda n}^0 = 2g_J \Gamma_{\lambda n} E^{-\frac{1}{2}} = \gamma_{\lambda n}, \quad \Gamma_{\lambda\mu}^{\mathrm{F}} = \tfrac{1}{2} \sum_{c(\mathrm{F})} \gamma_{\lambda c}\gamma_{\mu c}. \tag{21a, b, c}$$

Using equation (19) as an example, we have

$$\tfrac{1}{2}H_\lambda^{\mathrm{F}}/\gamma_{\lambda n} = \sum_{\mu \neq \lambda} \Gamma_{\mu\lambda}^{\mathrm{F}} \gamma_{\mu n}/(E_\mu - E_\lambda), \tag{22}$$

and the whole argument of Adler and Adler concerning the nonuniqueness of parameters is based upon the observation that, in equation (21c), we cannot specify the individual $\gamma_{\lambda c}$ when the number N_c of channels is greater than two. Adler and Adler did, in fact, give alternative solutions which yielded the same cross section in a number of special cases. However, the role of unitarity in this approximate version of the theory is obscured because the approximation itself violates unitarity to a slight degree.

Role of Unitarity

Unitarity essentially implies the condition

$$\mathrm{Im}\ T_{cc'} = \sum_{c''} T_{cc''} T_{c'c''}^*. \tag{23}$$

If we substitute the Kapur–Peierls form (8) into equation (23) and equate the residues of the resonance poles, we obtain

$$g_{\lambda c} = 2\mathrm{i} \sum_\mu g_{\mu c}^* X_{\lambda\mu}/(C_\mu^* - C_\lambda). \tag{24}$$

If we define the complex hermitian matrix **B** by

$$B_{\lambda\mu} = 2\mathrm{i}\, X_{\lambda\mu}/(C_\mu^* - C_\lambda) \tag{25}$$

then in matrix notation we have

$$\boldsymbol{g}_c = \mathbf{B}\boldsymbol{g}_c^* \quad \text{and} \quad \boldsymbol{g}_c^* = \mathbf{B}^*\boldsymbol{g}_c, \tag{26a, b}$$

from which we obtain

$$\mathbf{B}\mathbf{B}^* = \mathbf{I}. \tag{27}$$

We can associate a matrix $\mathbf{B}^{(x)}$ with each reaction by defining

$$B_{\lambda\mu}^{(x)} = 2\mathrm{i}\, X_{\lambda\mu}^{(x)}/(C_\mu^* - C_\lambda). \tag{28}$$

On denoting the hermitian conjugate by a dagger, we note also that

$$\mathbf{S}^{-1}\boldsymbol{g}_c = (\mathbf{S}^*)^{-1}\boldsymbol{g}_c^* = \mathbf{S}^\dagger \boldsymbol{g}_c^*, \tag{29}$$

so that we have

$$\mathbf{B} = \mathbf{S}\mathbf{S}^\dagger. \tag{30}$$

The matrix which complex-conjugates the Kapur–Peierls widths must also obey the condition (30) where $\mathbf{S}$ diagonalizes the level matrix.

In radiative capture channels we can write a random phase approximation as

$$\sum_{c(\gamma)} \gamma_{\nu c}\gamma_{\rho c} \approx \bar{\Gamma}_\gamma \delta_{\nu\rho}, \tag{31}$$

where $\bar{\Gamma}_\gamma$ is the average radiative width. Thus we obtain

$$X_{\lambda\mu}^{(\gamma)} = \sum_{c(\gamma)} \sum_{\nu\rho} \gamma_{\nu c} S_{\lambda\nu}\gamma_{\rho c} S_{\mu\rho}^* = \bar{\Gamma}_\gamma B_{\lambda\mu}. \tag{32}$$

Also equations (28) and (16) yield

$$\mathbf{B} = \mathbf{B}^{(n)} + \mathbf{B}^{(\mathrm{F})} + \mathbf{B}^{(\gamma)} \tag{33}$$

from which we obtain

$$X_{\lambda\mu}^{(\mathrm{F})} = \{\tfrac{1}{2}\mathrm{i}(C_\mu - C_\lambda^*) - \bar{\Gamma}_\gamma\} B_{\lambda\mu} - g_{\lambda n} g_{\mu n}^*. \tag{34}$$

The problem to be solved is, given a set of Adler–Adler resonance parameters which determine a cross section uniquely, how much information can be obtained about the Kapur–Peierls resonance parameters? From equation (14) we can determine the $g_{\lambda n}$ up to a sign, and so from equation (34) we must find either of the matrices $\mathbf{X}^{(\mathrm{F})}$ or $\mathbf{B}$. We assume that the average radiation width $\bar{\Gamma}_\gamma$ is known. For fissile materials, equation (15) then gives

$$G_\lambda^{(\gamma)} + \mathrm{i}\, H_\lambda^{(\gamma)} = \bar{\Gamma}_\gamma \sum_\mu X_{\lambda\mu}^{(n)} B_{\lambda\mu}/(C_\mu^* - C_\lambda) \tag{35}$$

and

$$G_\lambda^{(\mathrm{F})} + \mathrm{i}H_\lambda^{(\mathrm{F})} = \sum_\mu X_{\lambda\mu}^{(n)} X_{\lambda\mu}^{(\mathrm{F})}/(C_\mu^* - C_\lambda). \tag{36}$$

For N resonances, this represents $4N$ constraints upon $\mathbf{B}$ or $\mathbf{X}^{(\mathrm{F})}$. These are insufficient to determine any of the fission widths, and we regard these widths as the unknowns in the problem.

Now let us consider the effect of unitarity. We assume only one neutron channel. Equation (27) yields N^2 constraints while equations (26) give $2N(N_\mathrm{F}+1)$ constraints, where N_F is the number of fission channels. These constraints are not independent, and so we choose the greater number N^2. The equation

$$X_{\lambda\mu}^{(\mathrm{F})} = \sum_{c(\mathrm{F})} g_{\lambda c} g_{\mu c}^* \tag{37}$$

yields an additional N^2 conditions, so that in all we have $2N^2+4N$ constraints and only $2NN_F$ unknowns. The problem as posed, therefore, has no solution unless some of the constraints are redundant or relaxed. For example, the C_μ are not really independent variables but are intimately connected with the reduced widths $g_{\mu c}$ by way of equation (27). It follows that $2N^2+2N(2-N_F)$ redundancies must occur via these relations if the fission widths are to be determined.

The most sensible approach to this problem is to fit cross sections directly to the Kapur–Peierls form while using the unitary nature of the **T** matrix as a constraint upon the fit. Then all of the above conditions are automatically satisfied and Adler–Adler parameters can be derived rather than fitted directly.

A knowledge of **B** obtained in this way does not permit the determination of **S**. It is a consequence of the work of Adler and Adler (1972) that **S** is not a unique matrix and, for more than two fission channels, a number of such matrices can be defined which obey equation (30) and diagonalize a suitable level matrix. Another problem related to the above is, given a set of Kapur–Peierls parameters, can one find a unique set of Wigner–Eisenbud (1947) parameters?

References

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