A METHOD FOR INVERTING THE CHANNEL MATRIX IN R-MATRIX THEORY

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Abstract

A technique is presented for inverting the channel matrix which occurs in R-matrix theory. The collision matrix is expressed in a form which does not involve matrix inversions; it is evaluated by the application of a recurrence relation. The connection between this method and the level matrix formalism is examined.

I. Introduction

The resonance structure of nuclear reaction cross sections is usually studied by the R-matrix theory developed by Wigner and Eisenbud (1947) (Lane and Thomas 1958). In this theory there occurs the channel matrix, the inverse of which is required for the calculation of the collision matrix. When the number of reaction channels is large the inversion of the channel matrix can be carried out analytically only in the special case where the R-matrix is of rank one (Teichmann 1950; Newton 1952), as is the case when it contains one single level. The cross section is then given by the familiar Breit–Wigner single level formula.

The single level theory has enjoyed a great deal of success in its description of resonances for many nuclei, but there are nuclei, notably the fissiles, for which the single level formula has proved inadequate. Several multilevel theories have been developed which take into account the interference between resonances (Thomas 1955; Reich and Moore 1958; Vogt 1958). All these theories are based on a method for expressing the collision matrix in a form in which the channel matrix has been eliminated, and the problem of inverting the channel matrix is replaced by one of inverting the level matrix.

This paper presents an alternative approach to the problem of inverting the channel matrix. The collision matrix is expressed in a form which does not involve matrix inversions; it is obtained by the application of a relatively simple recurrence relation. The relationship between this method and the level matrix expansion is discussed and approximations for the collision matrix are derived.

II. Channel Matrix Inversion

The collision matrix $\mathbf{U}$ is connected with the R-matrix through the relation (Lane and Thomas 1958)

$$\mathbf{U} = \mathbf{\Omega}[\mathbf{I}+2\mathrm{i}\mathbf{P}^{\frac{1}{2}}(\mathbf{I}-\mathbf{R}\mathbf{L}^{0})^{-1}\mathbf{R}\mathbf{P}^{\frac{1}{2}}]\mathbf{\Omega}\,. \tag{1}$$

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$\mathbf{R}$ is a symmetric matrix with elements

$$R_{cc'} = \sum_{\lambda} \gamma_{\lambda c}\gamma_{\lambda c'}/(E_{\lambda}-E)\,, \tag{2}$$

where $\gamma_{\lambda c}$ and E_{λ} are real constants, while $\mathbf{\Omega}$, $\mathbf{L}^0$, and $\mathbf{P}$ are diagonal matrices with elements related by

$$\Omega_c = \exp(-\mathrm{i}\phi_c)\,, \qquad L_c^0 = S_c - B_c + \mathrm{i}P_c\,, \tag{3}$$

where, for channel c, ϕ_c is the hard-sphere scattering phase shift, S_c the level shift, P_c the penetration factor, and B_c a constant arising from the boundary conditions.

The central problem in calculating $\mathbf{U}$ is the determination of the matrix

$$\mathbf{S} = (\mathbf{I}-\mathbf{R}\mathbf{L}^0)^{-1}\mathbf{R}\,. \tag{4}$$

The present method for solving this problem is based on the well-known result (Lane and Thomas 1958) that, if

$$\mathbf{R} = \mathbf{R}_1 + \mathbf{R}_1'\,, \tag{5}$$

$\mathbf{S}$ can be expressed as a sum of two terms, one of them involving only $\mathbf{R}_1$ and the other involving both $\mathbf{R}_1$ and $\mathbf{R}_1'$. That is,

$$\begin{aligned} \mathbf{S} &= (\mathbf{I}-\mathbf{R}\mathbf{L}^0)^{-1}\mathbf{R} \\ &= (\mathbf{I}-\mathbf{R}_1\mathbf{L}^0)^{-1}\mathbf{R}_1 + (\mathbf{I}-\mathbf{R}_1\mathbf{L}^0)^{-1}(\mathbf{I}-\mathbf{R}_1'\mathbf{L}^{(1)})^{-1}\mathbf{R}_1'(\mathbf{I}-\mathbf{L}^0\mathbf{R}_1)^{-1}\,, \end{aligned} \tag{6}$$

where

$$\mathbf{L}^{(1)} = \mathbf{L}^0(\mathbf{I}-\mathbf{R}_1\mathbf{L}^0)^{-1}\,. \tag{7}$$

We note from equation (2) that the R-matrix is a sum over single level R-matrices,

$$\mathbf{R} = \sum_{\lambda} \mathbf{R}_{\lambda}\,. \tag{8}$$

Since each $\mathbf{R}_{\lambda}$ is a matrix of rank one, it follows that

$$(\mathbf{R}_{\lambda}\mathbf{L}^0)^2 = \mathbf{R}_{\lambda}\mathbf{L}^0\,\mathrm{trace}(\mathbf{R}_{\lambda}\mathbf{L}^0) \tag{9}$$

and therefore that

$$(\mathbf{I}-\mathbf{R}_{\lambda}\mathbf{L}^0)^{-1} = \mathbf{I} + \mathbf{R}_{\lambda}\mathbf{L}^0/\{1-\mathrm{trace}(\mathbf{R}_{\lambda}\mathbf{L}^0)\}\,. \tag{10}$$

Thus writing

$$\mathbf{R} = \mathbf{R}_1 + \sum_{\lambda \geqslant 2} \mathbf{R}_{\lambda} \tag{11}$$

and substituting in equation (6), we obtain

$$\mathbf{S} = \frac{\mathbf{R}_1}{1-\mathrm{trace}(\mathbf{R}_1\mathbf{L}^0)} + \left(\mathbf{I} + \frac{\mathbf{R}_1\mathbf{L}^0}{1-\mathrm{trace}(\mathbf{R}_1\mathbf{L}^0)}\right)\left(\mathbf{I}-\mathbf{R}_1'\mathbf{L}^{(1)}\right)^{-1}\mathbf{R}_1'\left(\mathbf{I} + \frac{\mathbf{L}^0\mathbf{R}_1}{1-\mathrm{trace}(\mathbf{R}_1\mathbf{L}^0)}\right), \tag{12}$$

where

$$\mathbf{L}^{(1)} = \mathbf{L}^0 + \mathbf{L}^0\mathbf{R}_1\mathbf{L}^0/\{1-\mathrm{trace}(\mathbf{R}_1\mathbf{L}^0)\}\,. \tag{13}$$

We may now write

$$\mathbf{R}_1' = \mathbf{R}_2+\mathbf{R}_2' \tag{14}$$

and use equation (6) again to expand the matrix $\mathbf{S}_1$, where

$$\mathbf{S}_1 = (\mathbf{I}-\mathbf{R}_1'\mathbf{L}^{(1)})^{-1}\mathbf{R}_1'. \tag{15}$$

This procedure can be repeated as many times as there are levels, or at least until enough levels have been included to allow the remainder to be treated as a constant background $\mathbf{R}_\infty$.

Thus, after eliminating k levels from the R-matrix, the elimination of the next level is achieved by using

$$(\mathbf{I}-\mathbf{R}_k'\mathbf{L}^{(k)})^{-1}\mathbf{R}_k' = \frac{\mathbf{R}_{k+1}}{1-T_{k+1,k}}+\left(\mathbf{I}+\frac{\mathbf{R}_{k+1}\mathbf{L}^{(k)}}{1-T_{k+1,k}}\right)$$

$$\times\left(\mathbf{I}-\mathbf{R}_{k+1}'\mathbf{L}^{(k+1)}\right)^{-1}\mathbf{R}_{k+1}'\left(\mathbf{I}+\frac{\mathbf{L}^{(k)}\mathbf{R}_{k+1}}{1-T_{k+1,k}}\right), \tag{16}$$

where

$$\mathbf{L}^{(k+1)} = \mathbf{L}^{(k)}+\mathbf{L}^{(k)}\mathbf{R}_{k+1}\mathbf{L}^{(k)}/(1-T_{k+1,k}) \tag{17}$$

and

$$T_{ij} = \mathrm{trace}(\mathbf{R}_i\mathbf{L}^{(j)}). \tag{18}$$

Therefore, if we write the R-matrix as a sum over N levels plus a background $\mathbf{R}_\infty$, we obtain eventually

$$\mathbf{S} = \frac{\mathbf{R}_1}{1-T_{10}}+\sum_{k=1}^{N-1}\left\{\prod_{i=1}^{k}\left(\mathbf{I}+\frac{\mathbf{R}_i\mathbf{L}^{(i-1)}}{1-T_{i,i-1}}\right)\right\}\frac{\mathbf{R}_{k+1}}{1-T_{k+1,k}}\left\{\prod_{i=k}^{1}\left(\mathbf{I}+\frac{\mathbf{L}^{(i-1)}\mathbf{R}_i}{1-T_{i,i-1}}\right)\right\}$$

$$+\left\{\prod_{i=1}^{N}\left(\mathbf{I}+\frac{\mathbf{R}_i\mathbf{L}^{(i-1)}}{1-T_{i,i-1}}\right)\right\}\left(\mathbf{I}-\mathbf{R}_\infty\mathbf{L}^{(N)}\right)^{-1}\mathbf{R}_\infty\left\{\prod_{i=N}^{1}\left(\mathbf{I}+\frac{\mathbf{L}^{(i-1)}\mathbf{R}_i}{1-T_{i,i-1}}\right)\right\}. \tag{19}$$

For the sake of simplicity we shall ignore the background term in (19) since there are adequate methods available for including the background when only a finite number of terms in the R-matrix are considered (Vogt 1960).

Equation (17) can be rewritten in the form

$$(\mathbf{L}^{(i)})^{-1}\mathbf{L}^{(i+1)} = \mathbf{I}+\mathbf{R}_{i+1}\mathbf{L}^{(i)}/(1-T_{i+1,i}). \tag{20}$$

Using this relation, the kth term on the right of (19) simplifies to

$$(\mathbf{L}^0)^{-1}\mathbf{L}^{(1)}(\mathbf{L}^{(1)})^{-1}\dots\mathbf{L}^{(k)}\{\mathbf{R}_{k+1}/(1-T_{k+1,k})\}\mathbf{L}^{(k)}\dots(\mathbf{L}^{(1)})^{-1}\mathbf{L}^{(1)}(\mathbf{L}^0)^{-1}$$

$$= (\mathbf{L}^0)^{-1}\mathbf{L}^{(k)}\{\mathbf{R}_{k+1}/(1-T_{k+1,k})\}\mathbf{L}^{(k)}(\mathbf{L}^0)^{-1},$$

so that (19) becomes

$$\mathbf{S} = (\mathbf{L}^0)^{-1}\sum_{k=0}^{N-1}\{\mathbf{L}^{(k)}\mathbf{R}_{k+1}\mathbf{L}^{(k)}/(1-T_{k+1,k})\}(\mathbf{L}^0)^{-1}. \tag{21}$$

This can be simplified even further by noting that, if we carry out a summation from $k = 0$ to $N-1$ on both sides of (17), we get

$$\mathbf{L}^{(N)} = \mathbf{L}^0 + \sum_{k=0}^{N-1} \mathbf{L}^{(k)}\mathbf{R}_{k+1}\mathbf{L}^{(k)}/(1-T_{k+1,k}). \tag{22}$$

Thus we obtain the following simple form

$$\mathbf{S} = (\mathbf{I}-\mathbf{R}\mathbf{L}^0)^{-1}\mathbf{R} = (\mathbf{L}^0)^{-1}(\mathbf{L}^{(N)}-\mathbf{L}^0)(\mathbf{L}^0)^{-1}. \tag{23}$$

The matrix $\mathbf{L}^{(N)}$ can be calculated from the recurrence relation (17) and therefore the calculation of $\mathbf{S}$ does not involve any matrix inversions.

III. Connection with Level Matrix Formalism

In the level matrix formalism (Lane and Thomas 1958) a particular element $S_{cc'}$ of $\mathbf{S}$ is expressed in the form

$$S_{cc'} = \{(\mathbf{I}-\mathbf{R}\mathbf{L}^0)^{-1}\mathbf{R}\}_{cc'} = \sum_{\lambda\mu} \gamma_{\lambda c}\gamma_{\mu c'}A_{\lambda\mu}, \tag{24}$$

where the matrix $\mathbf{A}$ is the inverse of the level matrix $\mathbf{C}$ which has elements

$$C_{\lambda\mu} = (E_\lambda - E)\delta_{\lambda\mu} - \xi_{\lambda\mu}, \tag{25}$$

where

$$\xi_{\lambda\mu} = \sum_c \gamma_{\lambda c}\gamma_{\mu c}L_c^0. \tag{26}$$

The element $S_{cc'}$ can be evaluated if the values of E_λ, $\gamma_{\lambda c}$, $\gamma_{\lambda c'}$, and $\xi_{\lambda\mu}$ are known for all λ and μ. If there are N levels, the number of parameters required to determine any one particular element of $\mathbf{S}$ is $\frac{1}{2}N(N+1)+3N$, which is independent of the number of channels.

On the other hand, if we wish to use the recurrence relation (17) to determine a given element $S_{cc'}$ then it is necessary to know the values of E_λ and $\gamma_{\lambda c}$ for all values of λ and c. In this case we require $N(M+1)$ parameters, where M is the number of channels. However, since the two methods are equivalent, there must be a means of calculating $L_{cc'}^{(N)}$ using only those parameters which occur in the level matrix formalism. A method is easily found by introducing the quantities $\beta_{\lambda c}^{(k)}$ and $\xi_{\lambda\mu}^{(k)}$, which are defined as

$$\beta_{\lambda c}^{(k)} = \sum_{c'} \gamma_{\lambda c'}L_{cc'}^{(k)} \tag{27}$$

and

$$\xi_{\lambda\mu}^{(k)} = \sum_c \gamma_{\lambda c}\beta_{\mu c}^{(k)} = \sum_{cc'} \gamma_{\lambda c}\gamma_{\mu c'}L_{cc'}^{(k)}. \tag{28}$$

For $k = 0$ these quantities are just the parameters which occur in the level matrix.

From equation (17) we have

$$L_{cc'}^{(n)} = L_{cc'}^{(n-1)} + (\mathbf{L}^{(n-1)}\mathbf{R}_n\mathbf{L}^{(n-1)})_{cc'}/\{1-\mathrm{trace}(\mathbf{R}_n\mathbf{L}^{(n-1)})\}. \tag{29}$$

However,

$$(\mathbf{L}^{(n-1)}\mathbf{R}_n\mathbf{L}^{(n-1)})_{cc'} = \beta_{nc}^{(n-1)}\beta_{nc'}^{(n-1)}/(E_n-E) \tag{30}$$

and

$$\mathrm{trace}(\mathbf{R}_n \mathbf{L}^{(n-1)}) = \xi_{nn}^{(n-1)}/(E_n - E), \tag{31}$$

and therefore

$$L_{cc'}^{(n)} = L_{cc'}^{(n-1)} + \beta_{nc}^{(n-1)} \beta_{nc'}^{(n-1)}/(E_n - E - \xi_{nn}^{(n-1)}). \tag{32}$$

If we multiply both sides of (32) by $\gamma_{n+1,c'}$ and carry out the summation over c' we find

$$\beta_{n+1,c}^{(n)} = \beta_{n+1,c}^{(n-1)} + \beta_{nc}^{(n-1)} \xi_{n+1,n}^{(n-1)}/(E_n - E - \xi_{nn}^{(n-1)}). \tag{33}$$

By repeating this procedure, this time multiplying throughout by γ_{kc}, we obtain

$$\xi_{n+1,k}^{(n)} = \xi_{n+1,k}^{(n-1)} + \xi_{nk}^{(n-1)} \xi_{n+1,n}^{(n-1)}/(E_n - E - \xi_{nn}^{(n-1)}). \tag{34}$$

We see then that starting only with the values of E_λ, $\beta_{\lambda c}^{(0)}$, $\beta_{\lambda c'}^{(0)}$, and $\xi_{\lambda\mu}^{(0)}$ we can use the recurrence relations (33) and (34) to determine $\beta_{nc}^{(n-1)}$, $\beta_{nc'}^{(n-1)}$, and $\xi_{nn}^{(n-1)}$, and thus $S_{cc'}$.

IV. Approximations

In the level matrix formalism, approximations for $\mathbf{S}$ are usually obtained by writing the level matrix $\mathbf{C}$ in the form (Schmidt 1966)

$$\mathbf{C} = \mathbf{D} + \boldsymbol{\xi}', \tag{35}$$

where $\mathbf{D}$ is the diagonal part of $\mathbf{C}$ and $\boldsymbol{\xi}'$ the off-diagonal part. Approximations for $\mathbf{S}$ are then found by the expansion

$$\mathbf{A} = \mathbf{D}^{-1} + \mathbf{D}^{-1}\boldsymbol{\xi}'\mathbf{D}^{-1} + \dots. \tag{36}$$

Instead of this procedure we can obtain $\mathbf{S}$ by using a perturbation method based on equation (22). As a first approximation we replace $\mathbf{L}^{(k)}$ by $\mathbf{L}^0$ on the right of (22) and obtain

$$\mathbf{L}^{(N)} \approx \mathbf{L}^0 + \sum_{k=0}^{N-1} \mathbf{L}^0 \mathbf{R}_{k+1} \mathbf{L}^0/(1 - T_{k+1,0}) \tag{37}$$

and hence

$$S_{cc'} \approx \sum_\lambda \gamma_{\lambda c}\gamma_{\lambda c'}/(E_\lambda - E - \xi_{\lambda\lambda}^0). \tag{38}$$

Exactly the same result is obtained by using only the first term on the right of (36) to calculate $\mathbf{S}$. A better approximation is obtained by substituting

$$\mathbf{L}^{(k)} \approx \mathbf{L}^0 + \sum_{i=0}^{k-1} \mathbf{L}^0 \mathbf{R}_{i+1} \mathbf{L}^0/(1 - T_{i+1,0}) \tag{39}$$

into (22) whence

$$\mathbf{S} = \sum_{k=0}^{N-1} \frac{\mathbf{L}^0\mathbf{R}_{k+1}\mathbf{L}^0}{1 - T_{k+1,k}} + \sum_{k=0}^{N-1}\sum_{i=0}^{k-1} \frac{\mathbf{L}^0\mathbf{R}_{k+1}\mathbf{L}^0\mathbf{R}_{i+1}\mathbf{L}^0 + \mathbf{L}^0\mathbf{R}_{i+1}\mathbf{L}^0\mathbf{R}_{k+1}\mathbf{L}^0}{(1 - T_{i+1,i})(1 - T_{k+1,k})}$$

$$+ \sum_{k=0}^{N-1}\sum_{i,j=0}^{k-1} \frac{\mathbf{L}^0\mathbf{R}_{i+1}\mathbf{L}^0\mathbf{R}_{k+1}\mathbf{L}^0\mathbf{R}_{j+1}\mathbf{L}^0}{(1 - T_{i+1,i})(1 - T_{k+1,k})(1 - T_{j+1,j})}. \tag{40}$$

In this approximation the traces $T_{k+1,k}$ must be calculated using $\mathbf{L}^{(k)}$ as given by equation (39). By approximating equation (40) further, we can obtain a result that is usually derived from the level matrix formalism. Thus, if we omit the third term on the right of (40) and replace $\mathbf{L}^{(k)}$ by $\mathbf{L}^0$ in the evaluation of the traces, we obtain

$$S_{cc'} \approx \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_{\lambda}-E-\xi^0_{\lambda\lambda}} + \sum_{\lambda} \sum_{\mu\neq\lambda} \frac{\gamma_{\lambda c}\gamma_{\mu c'}\,\xi^0_{\lambda\mu}}{(E_{\lambda}-E-\xi^0_{\lambda\lambda})(E_{\mu}-E-\xi^0_{\mu\mu})}. \tag{41}$$

This expression for $S_{cc'}$ is the same as that obtained from the level matrix formulation using the first two terms of (36). It should be noted that the analysis of resonances using a theory based on the expansion (36) will never give the correct position and total width of the resonances no matter how many terms are taken. This is because for a finite number of terms the poles of $\mathbf{A}$, and therefore also those in $\mathbf{S}$, are always at $E = E_{\lambda}-\xi_{\lambda\lambda}$, whereas their true positions are given by the eigenvalues of the level matrix. The present perturbation method does not have this problem since the traces in equation (40) are calculated using $\mathbf{L}^{(k)}$ given by (39).

V. Conclusions

We have seen how the channel matrix can be inverted so that the resulting expression for the collision matrix no longer involves matrix inversions. By examining the relation between this method and the more conventional method involving the level matrix, we have found that parameterization of the collision matrix in terms of level matrix parameters is still possible. It also appears that this method has some advantages over the level matrix formalism when it comes to finding approximations for the collision matrix.

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VII. References

Lane, A. M., and Thomas, R. G. (1958).—*Rev. mod. Phys.* **30**, 257.

Newton, T. D. (1952).—*Can. J. Phys.* **30**, 53.

Reich, C. W., and Moore, M. S. (1958).—*Phys. Rev.* **111**, 929.

Schmidt, J. J. (1966).—"Neutron Cross Sections for Fast Reactor Materials." Vol. 1. KFK120 (EANDC–E–35U). (Gesellschaft für Kernforschung: Karlsruhe.)

Teichmann, T. (1950).—*Phys. Rev.* **77**, 506.

Thomas, R. G. (1955).—*Phys. Rev.* **97**, 224.

Vogt, E. (1958).—*Phys. Rev.* **112**, 203.

Vogt, E. (1960).—*Phys. Rev.* **118**, 724.

Wigner, E. P., and Eisenbud, L. (1947).—*Phys. Rev.* **71**, 29.