REACTION MATRIX APPROACH TO THE INVERSE PROBLEM

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[Manuscript received 15 June 1971]

Abstract

The problem of inverting the calculation of cross sections to one of determining interaction potentials from cross sections is dealt with using the reaction matrix approach. The experimentally obtained resonance parameters are utilized to calculate constants which are coefficients of expansion of the potential in terms of known functions.

I. Introduction

A direct relationship between the scattering phase shift and the potential field responsible for the scattering process is of great value in the study of the physics of microscopic particles. Early work in this direction by Frodberg (1947) and Hylleraas (1948) consisted of expansion for the potential V in terms of s-wave phase shifts. Bargmann (1949) illustrated that there exists a class of phase equivalent solutions for V, which revealed that the former work lacked uniqueness in the solution, and Levinson (1949) showed that the ambiguity is related to the existence of a discrete spectrum. Marchenko (1950, 1952) proved that a sufficient set of parameters to determine V is given by the phase shift, the energies of all bound states, and the normalization constants. Further work by Holmberg (1952) and Jost and Kohn (1952) verified this conclusion.

A method of direct calculation of V from s-wave data was given by Gel'fand and Levitan (1951). Their method is mathematically most involved and does not seem to be particularly suited to numerical derivation of the potential. In the present paper, techniques are derived for resolving the scattering phase shift into components of the Wigner and Eisenbud (1947) matrix and then analysing the scattering problem by means of this matrix to obtain the interaction.

II. Reaction Matrix

We shall first consider the one-channel case. The radial wavefunction of the particle obeys (Preston 1965)

$$\frac{\mathrm{d}^2\psi_l(r)}{\mathrm{d}r^2}+\frac{2M}{\hbar^2}\left(E-V-\frac{l(l+1)}{2Mr^2}\right)\psi_l(r)=0\,, \tag{1}$$

where M is the reduced mass of the system, E the total energy, V the interaction potential, and l the orbital angular momentum. A radius $r=a$ is chosen at which V vanishes or is negligibly small. The $\mathscr{R}_l$ function is defined by

$$\psi_l(a)=\mathscr{R}_l(E)\,a\,(\mathrm{d}\psi_l/\mathrm{d}r)_{r=a}\,. \tag{2}$$

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Omitting the suffix l and putting $\hbar = 1$ we obtain for each partial wave

$$\psi = C(I - SO), \tag{3}$$

where I is the incoming wavefunction, O the outgoing wavefunction, and C a constant. Substitution of (3) into (2) gives

$$S = \Omega^2(1 - L^*\mathscr{R})/(1 - L\mathscr{R}), \quad \Omega^2 = I/O, \quad L = aO'(a)/O(a). \tag{4}$$

Equation (1) is then solved across the interior region $r < a$ where it has discrete eigenvalues E_λ when the boundary conditions (see Preston 1965)

$$(\mathrm{d}U_\lambda/\mathrm{d}r)_{r=a} = (B/a)U_\lambda(a) \tag{5}$$

are satisfied and the $U_\lambda(r)$ form an orthonormal set in the interval $0 \leqslant r \leqslant a$, that is,

$$\int_0^a \mathrm{d}r\, U_\lambda\, U_{\lambda'} = \delta_{\lambda\lambda'}. \tag{6}$$

The physical solution of (1) across the interior has a continuum of eigenvalues E and does not necessarily obey the boundary conditions (5). However, we can use the expansion

$$\psi(r) = \sum_\lambda A_\lambda\, U_\lambda(r), \qquad V\psi = \sum_\lambda A_\lambda\, V_\lambda(r)\, U_\lambda(r), \tag{7}$$

together with Green's theorem to show that

$$A_\lambda = \frac{1}{2M}\frac{U_\lambda(a)}{E_\lambda - E}\left(\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)_a (1 - B\mathscr{R}) \tag{8}$$

and hence that

$$\mathscr{R} = R/(1 + BR),$$

with

$$R = \frac{1}{2Ma}\sum_\lambda \frac{U_\lambda^2(a)}{E_\lambda - E} = \sum_\lambda \frac{\gamma_\lambda^2}{E_\lambda - E}. \tag{9}$$

However, across the same region we can solve (1) for $V = 0$ with the boundary conditions (5) to obtain an orthonormal set of free particle wavefunctions $W_\mu(r)$. We then have the equations

$$(\nabla_r^2 + 2M(E_\lambda - V_\lambda))U_\lambda = 0, \qquad (\nabla_r^2 + 2ME_{\mu 0})W_\mu = 0, \tag{10a, b}$$

where

$$\nabla_r^2 = \partial^2/\partial r^2 - l(l+1)/r^2$$

and the $E_{\mu 0}$ are the discrete eigenvalues obtained from W_μ. We can thus expand U_λ and $V_\lambda U_\lambda$ into the Dini series (Erdelyi 1953)

$$U_\lambda(r) = \sum_\mu B_{\lambda\mu}\, W_\mu(r), \qquad V_\lambda\, U_\lambda(r) = \sum_\mu V_{\lambda\mu}\, W_\mu(r). \tag{11a, b}$$

From Green's theorem, it follows that

$$W_\mu(a)\,U'_\lambda(a) - U_\lambda(a)\,W'_\mu(a) + 2M(E_\lambda - E_{\mu 0})B_{\lambda\mu} - 2MV_{\lambda\mu} = 0\,, \tag{12}$$

the prime denoting differentiation with respect to r, and so with the boundary conditions

$$W'_\mu(a)/W_\mu(a) = U'_\lambda(a)/U_\lambda(a) = B/a \tag{13}$$

we have

$$(E_\lambda - E_{\mu 0})B_{\lambda\mu} = V_{\lambda\mu}\,, \tag{14}$$

or in Dirac notation

$$\langle\lambda\,|\,V\,|\,\mu\rangle/\langle\lambda\,|\,\mu\rangle = E_\lambda - E_{\mu 0}\,. \tag{15}$$

More generally

$$(E_\lambda - E_{\mu 0})B_{\lambda\mu} = V_{\lambda\mu} - V^0_{\lambda\mu}\,, \tag{16}$$

where $V^0_{\lambda\mu}$ is the matrix derived from using a reference potential V^0, showing that the energy separation in eigenvalues is proportional to the matrix element of the difference in interaction potentials taken between the corresponding eigenstates.

Equation (16) illustrates that the shift in the location of the free particle pole sites when interactions are turned on is directly proportional to the matrix elements of the potential taken between the free particle state and the state in the presence of the interaction. It will now be shown how this interaction can be found. It follows that in order to have uniform convergence of the series (11b)

$$\left(\frac{\mathrm{d}(V_\lambda\,U_\lambda)}{\mathrm{d}r}\right)_a = \frac{B}{a}\left(V_\lambda\,U_\lambda\right)_a\,,$$

that is,

$$\left(\frac{\mathrm{d}V_\lambda}{\mathrm{d}r}\,.\,U_\lambda\right)_a = 0\,. \tag{17}$$

III. Algebraic Analogue of Schrödinger's Equation

In this section the reaction matrix analogue of Schrödinger's equation is derived. Although this equation is unnecessary to prove the validity of the inversion procedure, it does illustrate that an algebraic equivalent to Schrödinger's equation exists and gives a quantitative picture of how the matrix potential $V_{\lambda\mu}$ shifts the pole sites in the free particle spectrum to those of the spectrum in the presence of interactions. It was felt that this property was sufficiently interesting in itself to justify the inclusion of this section.

The function $\mathscr{R}$ is defined by

$$\mathscr{R} = R/(1+BR) = \psi(a)/a\psi'(a)\,,$$

which takes account of the second boundary condition in (5).

The equation for the scattering state can be written for each eigenstate of l (Corinaldesi and Strocchi 1963) in terms of the Bessel functions $J_\nu(kr)$ as

$$\psi(r) = (\tfrac{1}{2}\pi kr)^{\frac{1}{2}}\,J_{l+\frac{1}{2}}(kr) - 2M\int_0^\infty K(r,r')\,V(r')\,\psi(r')\,\mathrm{d}r'\,, \tag{18}$$

where, for $r' > r$,

$$K(r,r') = \tfrac{1}{2}\pi(rr')^{\frac{1}{2}} J_{l+\frac{1}{2}}(kr)\{(-1)^l J_{-l-\frac{1}{2}}(kr') + \mathrm{i} J_{l+\frac{1}{2}}(kr')\},$$

r' and r being interchanged for $r' < r$. The wavefunction ψ has asymptotic behaviour

$$\psi \sim \exp(\mathrm{i}\delta)\sin(kr - \tfrac{1}{2}l\pi + \delta_l) \tag{19}$$

for large r. It is more convenient to renormalize ψ by the relation

$$\psi(r) = \exp(\mathrm{i}\delta)\,\Psi(r)/\cos\delta, \tag{20}$$

which obeys the same equation as $\psi(r)$ and similar expansions to (7) and has kernel

$$K(r,r') = \tfrac{1}{2}(-1)^l \pi(rr')^{\frac{1}{2}} J_{l+\frac{1}{2}}(kr) J_{-l-\frac{1}{2}}(kr'), \qquad r' > r, \tag{21}$$

with r and r' interchanged for $r' < r$. Assuming that

$$\operatorname*{Lim}_{r\to a} V(r) = 0 \qquad \text{and} \qquad \operatorname*{Lim}_{r\to a} V'(r) = 0, \tag{22}$$

we find

$$\Psi(a) = \mathscr{S}(a) - \mathscr{C}(a)\,(2M/k)\int_0^a \mathscr{S}(r')\,V(r')\,\Psi(r')\,\mathrm{d}r', \tag{23}$$

where we use the non-conventional definitions

$$\mathscr{S}_l(r) = (\tfrac{1}{2}\pi kr)^{\frac{1}{2}} J_{l+\frac{1}{2}}(kr), \qquad \mathscr{C}_l(r) = (\tfrac{1}{2}\pi kr)^{\frac{1}{2}}(-1)^{l+1} J_{-l-\frac{1}{2}}(kr),$$

and

$$\Psi'(a) = \mathscr{S}'(a) - \mathscr{C}'(a)\,(2M/k)\int_0^a \mathscr{S}(r')\,V(r')\,\Psi(r')\,\mathrm{d}r'. \tag{24}$$

Let

$$\mathscr{K}(k) = (2M/k)\int_0^a \mathscr{S}(r')\,V(r')\,\Psi(r')\,\mathrm{d}r' = \tan\delta \tag{25}$$

be the reactance matrix. Then

$$\mathscr{R}(k) = \frac{\Psi(a)}{a\Psi'(a)} = \frac{\mathscr{S}(a) - \mathscr{C}(a)\mathscr{K}(k)}{a\{\mathscr{S}'(a) - \mathscr{C}'(a)\mathscr{K}(k)\}}$$

and therefore

$$\mathscr{K}(k) = \frac{\mathscr{S}(a) - a\mathscr{R}(k)\,\mathscr{S}'(a)}{\mathscr{C}(a) - a\mathscr{R}(k)\,\mathscr{C}'(a)}. \tag{26}$$

The quantity on the right is known, since $\mathscr{S}$ and $\mathscr{C}$ are given and $\mathscr{R}$ is determined from experiment. However, we now choose

$$\Psi = \sum_\lambda A_\lambda U_\lambda(r), \qquad \mathscr{S} = \sum_\mu b_\mu W_\mu(r), \tag{27}$$

where the b_μ and W_μ are known and A_λ and U_λ unknown. Therefore

$$\mathscr{K}(k) = (2M/k)\langle \mathscr{S} \mid V \mid \Psi\rangle = (2M/k)\sum_\lambda \sum_\mu A_\lambda b_\mu \langle \lambda \mid V \mid \mu\rangle. \tag{28}$$

From equations (7) and (8) and (9), with

$$A_\lambda = \frac{U_\lambda(a)\,\Psi'(a) - \Psi(a)\,U'_\lambda(a)}{2M(E_\lambda - E_{\mu 0})} = \left(\frac{\Psi'(a)}{\Psi(a)} - \frac{U'_\lambda(a)}{U_\lambda(a)}\right)\frac{U_\lambda(a)\,\Psi(a)}{2M(E_\lambda - E_{\mu 0})}$$

$$= \frac{1}{aR}\frac{1}{2M}\frac{U_\lambda(a)}{E_\lambda - E}\Psi(a) \tag{29}$$

and similarly

$$b_\mu = \frac{1}{aR_0}\frac{1}{2M}\frac{W_\mu(a)}{E_{\mu 0} - E}\mathscr{S}(a) \tag{30}$$

(R_0 being the free particle version of (9)), we get the function

$$I(k) = \mathscr{K}(k)/\Psi(a)\,\mathscr{S}(a) = \sum_\lambda \sum_\mu F_{\lambda\mu}\langle\lambda\,|\,V\,|\,\mu\rangle, \tag{31}$$

where

$$F_{\lambda\mu} = \frac{1}{a^2 R R_0}\frac{1}{(2M)^2}\frac{U_\lambda(a)\,W_\mu(a)}{(E_\lambda - E)(E_{\mu 0} - E)}. \tag{32}$$

Let us evaluate $I(k)$. We have

$$I(k) = \frac{\mathscr{S} - a\mathscr{R}\mathscr{S}'}{\mathscr{C} - a\mathscr{R}\mathscr{C}'}\frac{1}{\mathscr{S}(\mathscr{S} - \mathscr{C}\mathscr{K})} = \frac{\mathscr{S} - a\mathscr{R}\mathscr{S}'}{\mathscr{S}(\mathscr{S}\mathscr{C}' - \mathscr{C}\mathscr{S}')}\frac{1}{a\mathscr{R}}. \tag{33}$$

However, $\mathscr{S}$ and $\mathscr{C}$ satisfy the Wronskian relation

$$\mathscr{S}\mathscr{C}' - \mathscr{C}\mathscr{S}' = k. \tag{34}$$

Hence

$$I(k) = \frac{1}{ka\mathscr{R}} - \frac{\mathscr{S}'}{k\mathscr{S}}$$

$$= \frac{1}{ka}\left(\frac{1}{\mathscr{R}} - \frac{1}{\mathscr{R}_0}\right) = \frac{1}{ka}\left(\frac{1}{R} - \frac{1}{R_0}\right) \tag{35}$$

and we find

$$\frac{1}{ka}\left(\frac{1}{R} - \frac{1}{R_0}\right) = \frac{1}{a^2 R R_0 k}\left(\frac{1}{2M}\right)^2 \sum_\lambda \sum_\mu \frac{U_\lambda(a)\,W_\mu(a)}{(E_\lambda - E)(E_{\mu 0} - E)}\langle\lambda\,|\,V\,|\,\mu\rangle,$$

that is,

$$R = R_0 - \sum_\lambda \sum_\mu \frac{\gamma_\lambda\,\delta_\mu}{(E_\lambda - E)(E_{\mu 0} - E)}V_{\lambda\mu}, \tag{36}$$

where

$$R = \sum_\lambda \frac{\gamma_\lambda^2}{E_\lambda - E}, \quad R_0 = \sum_\mu \frac{\delta_\mu^2}{E_{\mu 0} - E}, \quad \gamma_\lambda^2 = \frac{U_\lambda^2(a)}{2Ma}, \quad \delta_\mu^2 = \frac{W_\mu^2(a)}{2Ma}. \tag{37}$$

Equation (36) is the R-matrix analogue of the scattering state equation (18). Its algebraic solution tells us the matrix elements $\langle\lambda\,|\,V\,|\,\mu\rangle$ from which the potential can be reconstructed.

IV. Solutions to R-state Equation

By equating poles on the left and right of (36), we find from the residues

$$\gamma_\lambda = \sum_\mu \frac{V_{\lambda\mu}\delta_\mu}{E_\lambda - E_{\mu 0}}, \qquad \delta_\mu = \sum_\lambda \frac{V_{\lambda\mu}\gamma_\lambda}{E_\lambda - E_{\mu 0}} = \sum_\lambda \frac{\tilde{V}_{\mu\lambda}\gamma_\lambda}{E_\lambda - E_{\mu 0}}, \tag{38}$$

where the tilde denotes transposition. However, we note from equation (15) that these may be written as

$$\gamma_\lambda = B_{\lambda\mu}\delta_\mu, \qquad \delta_\mu = B_{\lambda\mu}\gamma_\lambda. \tag{39}$$

If the functions $U_\lambda(r)$ and $W_\mu(r)$ are to satisfy the closure relations

$$\sum_\lambda U_\lambda(r)\,U_\lambda(r') = \sum_\mu W_\mu(r)\,W_\mu(r') = \delta(r-r'),$$

then we must have

$$B_{\lambda\mu}B_{\lambda\mu'} = \delta_{\mu\mu'} \qquad \text{and} \qquad B_{\lambda\mu}B_{\lambda'\mu} = \delta_{\lambda\lambda'}. \tag{40}$$

It follows that the matrix

$$B_{\lambda\mu} = \langle\lambda\,|\,\mu\rangle$$

must be unitary and that

$$\sum_\lambda U_\lambda^2(a) = \sum_\mu W_\mu^2(a). \tag{41}$$

One does not require the R-state equation to prove that $B_{\lambda\mu}$ is a unitary matrix. If we write

$$U_\lambda(r) = \sum_\mu B_{\lambda\mu}W_\mu(r), \qquad W_\rho(r) = \sum_\sigma G_{\rho\sigma}U_\sigma(r), \tag{42a, b}$$

where the matrix $\mathbf{G}$ is the inverse of $\mathbf{B}$, then multiplying (42a) by $W_{\mu'}(r)$ and (42b) by $U_{\sigma'}(r)$, integrating each over the range $0 \leqslant r \leqslant a$, and using the orthonormality conditions, we obtain

$$B_{\lambda\mu} = \int_0^a U_\lambda(r)\,W_\mu(r)\,\mathrm{d}r, \qquad G_{\rho\sigma} = \int_0^a W_\rho(r)\,U_\sigma(r)\,\mathrm{d}r$$

and therefore

$$B_{\lambda\mu} = G_{\mu\lambda},$$

so that the inverse of $\mathbf{B}$ is its transpose. Accordingly

$$W_\rho(r) = \sum_\lambda G_{\rho\lambda}U_\lambda(r) = \sum_\lambda\sum_\mu G_{\rho\lambda}B_{\lambda\mu}W_\mu(r).$$

Multiplying both sides by $W_\sigma(r)$ and using the orthonormality conditions again, we find

$$\delta_{\rho\sigma} = \sum_\lambda\sum_\mu G_{\rho\lambda}B_{\lambda\mu}\delta_{\mu\sigma} = \sum_\lambda B_{\lambda\rho}B_{\lambda\sigma},$$

that is,

$$\mathbf{B}^{\sim}\,\mathbf{B} = \mathbf{I}$$

and $\mathbf{B}$ is unitary.

The interaction therefore has the character of a rotation which alters a vector of components $W_\mu(a)$ to a vector of components $U_\lambda(a)$. In the case of a square well, the eigenfunctions U_λ are the same as for the free particle case. In this instance

$$B_{\lambda\mu} = \delta_{\lambda\mu}$$

and

$$V_{\lambda\mu} = \langle\lambda \mid V \mid \mu\rangle = (E_\lambda - E_{\mu 0})\delta_{\lambda\mu} = -\mid V_0 \mid \delta_{\lambda\mu} \tag{43}$$

and only a pole shift V_0 occurs, with no rotation of the eigenfunction vector $W_\mu(a)$.

The numerical technique of solving for $V_{\lambda\mu}$ with a finite number of poles is as follows. (1) First choose the background such that the poles have residues obeying (41); the vectors are then of the same length. (2) Define a series of rotations $\boldsymbol{\Omega}_i$ of the type

$$\boldsymbol{\Omega}_1 = \begin{bmatrix} \cos\theta_1 & -\sin\theta_1 & . & . \\ \sin\theta_1 & \cos\theta_1 & . & . \\ . & . & . & . \\ . & . & . & . \end{bmatrix}, \qquad \boldsymbol{\Omega}_2 = \begin{bmatrix} 1 & . & . & . \\ . & \cos\theta_2 & -\sin\theta_2 & . \\ . & \sin\theta_2 & \cos\theta_2 & . \\ . & . & . & . \end{bmatrix},$$

and so on, with

$$\cos\theta_i = W_{i+1} \Big/ \left(\sum_1^{i+1} W_k^2\right)^{\frac{1}{2}}, \qquad W_i = W_i(a), \qquad U_i = U_i(a), \tag{44}$$

which reduces to the vector

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ . \\ . \\ (\Sigma\, W_i^2)^{\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ . \\ . \\ (\Sigma\, U_k^2)^{\frac{1}{2}} \end{bmatrix}. \tag{45}$$

(3) Then apply a reverse series of rotations $\overline{\boldsymbol{\Omega}}_j$,

$$\cos\bar{\theta}_j = U_{j+1} \Big/ \left(\sum_1^{j+1} U_k^2\right)^{\frac{1}{2}},$$

which builds up the vector U_λ. The product of these two sets of rotations is the required matrix transformation, giving

$$\mathbf{B} = \prod_i \boldsymbol{\Omega}_i \prod_j \bar{\boldsymbol{\Omega}}_j \tag{46}$$

and finally, from equations (11),

$$V_\lambda(r) = \left(\sum_\mu V_{\lambda\mu} W_\mu(r)\right) \Big/ \left(\sum_\mu B_{\lambda\mu} W_\mu(r)\right), \tag{47}$$

where for a lamellar potential $V_\lambda = V_{\lambda+1} = V_{\lambda+2} \ldots$. For an energy-dependent potential, V_λ will be a function of λ and the correct potential is

$$V(r,E) = \left(\sum_\lambda \sum_\mu A_\lambda(E)\, V_{\lambda\mu}\, W_\mu(r)\right) \Big/ \left(\sum_\lambda \sum_\mu A_\lambda(E)\, B_{\lambda\mu}\, W_\mu(r)\right). \tag{48}$$

Following the above derivation for the multichannel case, one arrives after much tedious manipulation at the scattering R-state equation

$$R_{cc'} = R^0_{cc'} - \frac{\hbar^2}{2M(a_c a_{c'})^{\frac{1}{2}}} \sum_{\lambda,\mu,c''} \frac{W_{\mu c}\, U_{\lambda c''}}{(E_{\mu 0} - E)(E_\lambda - E)} \langle \mu c \mid V \mid \lambda c'' \rangle \tag{49}$$

from which the matrix potential that couples the channels can be evaluated. In equation (49) we have

$$R^0_{cc'} = (W_{\mu c}/a W'_{\mu c})\delta_{cc'}\,. \tag{50}$$

Such a reaction matrix makes no contribution to the off-diagonal elements of the scattering matrix.

Bargmann (1949) first showed the lack of uniqueness of the inverse reaction problem and this is manifested in the above procedure by the fact that there are $\frac{1}{2}(n^2-n)$ spare degrees of freedom in the $n \times n$ unitary matrix $B_{\lambda\mu}$.

V. Basic Generating Matrix

To find some simple basic form, we postulate a bilinear expression

$$B_{\lambda\mu} = AU_\lambda(a)\, W_\mu(a) + BU_\mu(a)\, W_\lambda(a) + CU_\lambda(a)\, U_\mu(a) + DW_\lambda(a)\, W_\mu(a) + F\delta_{\lambda\mu} \tag{51}$$

and after substituting into equations (39) and (40) we find that

$$A = B = -C = -D = \left(\sum_\lambda U^2_\lambda(a) - \sum_\lambda U_\lambda(a)\, W_\lambda(a)\right)^{-1},$$

in which case

$$B_{\lambda\mu} = A\{U_\lambda(a)\, W_\mu(a) + U_\mu(a)\, W_\lambda(a) - U_\lambda(a)\, U_\mu(a) - W_\lambda(a)\, W_\mu(a)\} + \delta_{\lambda\mu} \tag{52}$$

and $\mathbf{B}$ is a symmetric matrix. It follows that $\mathbf{B}$ is a solution of

$$\mathbf{B}^2 = \mathbf{I}\,. \tag{53}$$

VI. Numerical Approximations

When evaluating potentials from a given set of reaction matrix parameters, one is given only a finite number of poles E_λ and widths γ_λ that have been evaluated by a least squares fit to the phase shifts. A useful device which gives excellent approximations to the potential is to assume that the interaction tends to zero for energies well away from the region of interest. The method is as follows.

(1) Firstly, after calculating the $U_\lambda(a)$ one has n such poles and n corresponding free particle poles. One assumes

$$R = \sum_1^n \frac{\gamma_\lambda^2}{E_\lambda - E} + \frac{\gamma_{n+1}^2}{E_{n+1} - E} + R_0 - \sum_1^n \frac{\delta_\mu^2}{E_{\mu 0} - E}. \tag{54}$$

where R_0 is the free particle reaction matrix which can be evaluated analytically.

(2) The parameter γ_{n+1}^2 is calculated as

$$\gamma_{n+1}^2 = \sum_1^{n+1} \delta_\mu^2 - \sum_1^n \gamma_\lambda^2,$$

which ensures unitarity. E_{n+1} is then found from (54).

(3) The wavefunctions are then defined as

$$\Psi = \sum_\lambda \sum_\mu A_\lambda B_{\lambda\mu} W_\mu(r) + \Psi_0 - \sum_\lambda \sum_\mu A_\lambda^0 b_\mu W_\mu(r),$$

where Ψ_0 is the free particle wavefunction and A_λ^0 the free particle equivalent to A_λ.

These approximations have been tested successfully. They are necessary because one does not know details of the poles which contribute to the background constant term in the reaction matrix.

In programs written for the IBM 360/50 computer at the AAEC, trial sets of phase shifts were obtained and used to give a least squares fit to the reaction matrix as a sum of poles plus background. The parameters obtained were constrained to give a unitary **B** matrix, with a free particle or square well spectrum of poles outside the range examined. The potentials obtained reproduced the phase shifts when the Schrödinger equation was integrated, to better than four decimal places. This work has been completed, and details of the calculations and computer programs are available from the author. In practice, the use of background spectra amounts to using an infinite number of the U_λ and W_μ, but the sums over the background are carried out analytically, as shown above.

In conclusion, the procedure given here for obtaining the interaction component of the wave equation from scattering and reaction data analysed into *R*-matrix components is relatively simple and is easy to apply in numerical determinations of the interaction.

VII. Acknowledgments

The author thanks Dr. B. Clancy, Dr. W. K. Bertram, and Mr. E. Clayton for many interesting discussions, and Dr. G. Derrick for valuable criticism.

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