

SOLUTION OF THE INVERSE REACTION PROBLEM FOR COMPLEX POTENTIALS

By W. K. BERTRAM* and J. L. COOK*

[Manuscript received 26 November 1971]

Abstract

A method is given for solving the inverse reaction problem to obtain complex potentials as in the optical model of the nucleus. The method reproduces reaction data to the accuracy with which the reaction matrix can be least squares fitted to a sum of simple poles. The method couples multichannel phase shifts in such a way as to give the correct complex single-channel phase shift.

I. INTRODUCTION

Previous work by Cook (1970, 1972) has shown that, given the complex phase shifts in each channel of a reaction, a set of real channel wavefunctions and potentials can be evaluated which reproduces the phase shifts to the accuracy with which the reaction matrix can be least squares fitted to a sum of poles. This formulation can be generalized to derive an equivalent alternative theory which uses complex potentials as in the optical model (Preston 1962). Traditionally, the absence of uniqueness has been overcome by selecting trial potentials which reproduce the data satisfactorily, with the requirements upon the potentials that they have the smallest number of maxima and minima possible and can be represented by a few elementary mathematical functions. This method appears plausible in that it assumes that the experimental evidence will be insufficient to permit the calculation of a unique potential and therefore that the human investigator is entitled to choose potentials which are quickly evaluated.

The present authors do not wholly subscribe to the above view. Firstly, the lack of data concerning the behaviour of phase shifts in all channels except the elastic channels has prevented the study of systematic relationships between channels. Such a study could reveal a sufficient number of new rules to permit unique solutions. Secondly, an investigation of the shapes of potentials allows the possibility of recognizing physical characteristics known from other experiments. Thirdly, plausible physical models of the structure of the scattering target, which have sufficient detail to remove the necessary degrees of freedom, can be constructed; this is illustrated in Section IV with a well-known example. Such models are essentially guesses of the assumed missing rules.

One must also answer the criticism that the traditional calculation makes use of the principle that if a set of alternative hypotheses leads to the same conclusion, one should choose the simplest member of the set. Since the forward, i.e. potential to phase shift, calculation is quite adequate, why attempt the inverse calculation?

* AEC Research Establishment, Private Mail Bag, Sutherland, N.S.W. 2232.

Our answer is that we have chosen even simpler initial data, namely the experimentally measured cross sections. Furthermore, when proceeding with the inverse calculation, the above simplicity criterion was applied. Specifically, in the single-channel calculation (Cook 1970, 1972) the simplest form for a particular unitary matrix was chosen to remove the non-uniqueness. In other respects the inverse calculation is comparable in speed and simplicity to the forward one, and there is little to choose between the two approaches in this regard.

A further peculiarity of the forward and inverse calculations is that if one chooses a trial potential, calculates the phase shift, and then applies the inverse method to the latter, the trial potentials are generally not reproduced. This is because the simplest unitary transformation matrix does not often lead to the simplest potential which reproduces the phase shift.

II. OPTICAL MODEL

Before giving an account of how a complex potential can be determined, we must consider the formal theory of the optical model in order to establish exactly the experimental information that is required for the calculation. The basic radial wave equation for the optical model wavefunction U_{cl} for the incident channel c and orbital angular momentum l is (Preston 1962)

$$d^2 U_{cl}/dr^2 + \{k_c^2 - v_c - l(l+1)/r^2\} U_{cl} = 0. \quad (1)$$

For simplicity we assume the bombarding particles to be neutrons. The more general theory containing Coulomb effects is not difficult to derive. This wavefunction has the asymptotic form

$$U_{cl} \xrightarrow{(r \rightarrow \infty)} \mathcal{D}_{cl} \left[\{1 + \exp(-2\beta_{cl})\} \sin(k_c r - \frac{1}{2}l\pi + \alpha_{cl}) + i\{1 - \exp(-2\beta_{cl})\} \cos(k_c r - \frac{1}{2}l\pi + \alpha_{cl}) \right], \quad (2)$$

where \mathcal{D}_{cl} is an arbitrary complex constant and α_{cl} and β_{cl} are the real and imaginary parts of the phase shift respectively, with $\delta_{cl} = \alpha_{cl} + i\beta_{cl}$.

Neglecting spin for the present, the cross sections are:

elastic cross section

$$\sigma_{cc} = (2\pi/k_c^2) \sum_l (2l+1) |1 - \exp(+2i\delta_{cl})|^2, \quad (3a)$$

absorption cross section

$$\sigma_{ca} = (\pi/k_c^2) \sum_l (2l+1) \{1 - \exp(-4\beta_{cl})\}, \quad (3b)$$

total cross section

$$\sigma_{ct} = (2\pi/k_c^2) \sum_l (2l+1) [1 - \text{Re}\{\exp(+2\delta_{cl})\}]. \quad (3c)$$

Let us suppose, for the sake of simplicity that there are two channels in the reaction. The generalization to many channels is straightforward. We may associate with the cross sections a two-channel S matrix

$$S_{cc'} \equiv \begin{pmatrix} S_{11} & S_{12} \\ S_{12} & S_{22} \end{pmatrix}$$

such that

$$S_{11} = \exp(+2i\delta_1), \quad |S_{12}|^2 = 1 - \exp(-4\beta_1), \quad S_{22} = \exp(+2i\delta_2). \quad (4)$$

Although it is almost never experimentally realizable, we shall assume that the analysis of angular distributions in all channels has permitted the determination of all complex phase shifts. Means of overcoming deficiencies in experimental information are indicated in Section IV.

The \mathbf{T} matrix is defined as

$$\mathbf{T} = (\mathbf{S} - \mathbf{I})/2i, \quad (5)$$

while the reduced transition matrix \mathbf{T}' is defined by the equation

$$\mathbf{T} = (\mathbf{\Omega}^2 - \mathbf{I})/2i + \mathbf{\Omega} \mathbf{T}' \mathbf{\Omega}, \quad (6)$$

where $\mathbf{\Omega}$ is the diagonal matrix (Lane and Thomas 1958)

$$\mathbf{\Omega} = \begin{pmatrix} \exp(-i\theta_{1l}) & 0 \\ 0 & \exp(-i\theta_{2l}) \end{pmatrix} \quad (7)$$

and θ_1 and θ_2 are the hard sphere phase shifts for channels 1 and 2. Since the \mathbf{S} matrix is unitary and symmetric it can be readily shown that the \mathbf{T}' matrix must be of the form

$$\mathbf{T}' = \frac{1}{2i} \begin{pmatrix} \eta \exp(2i\alpha'_{1l}) - 1 & (1 - \eta^2)^{\frac{1}{2}} \exp(2i\phi_l) \\ (1 - \eta^2)^{\frac{1}{2}} \exp(2i\phi_l) & -\eta \exp\{2i(2\phi_l - \alpha'_{1l})\} - 1 \end{pmatrix}, \quad (8)$$

where $\eta = \exp(-2\beta_{1l})$, ϕ_l is an independent function, and the reduced phase shifts are $\alpha'_{cl} = \alpha_{cl} - \theta_{cl}$. These are required to calculate the potential using Cook's (1970, 1972) calculation.

In solving the inverse reaction problem, one associates a real channel wavefunction ψ_{cl} with each phase shift δ_{cl} such that each ψ_{cl} obeys Schrödinger's equation,

$$\frac{d^2\psi_{1l}}{dr^2} + \left(k_1^2 - V_1 - \frac{l(l+1)}{r^2} \right) \psi_{1l} = 0, \quad \frac{d^2\psi_{2l}}{dr^2} + \left(k_2^2 - V_2 - \frac{l(l+1)}{r^2} \right) \psi_{2l} = 0. \quad (9)$$

ψ_{1l} and ψ_{2l} have the asymptotic forms

$$\psi_{1l} \rightarrow C_{1l} \sin(k_1 r - \frac{1}{2}l\pi + \alpha_{1l}), \quad \psi_{2l} \rightarrow C_{2l} \sin(k_2 r - \frac{1}{2}l\pi + \alpha_{2l}). \quad (10)$$

It can be shown that ψ_{1l} and ψ_{2l} are not independent of each other but are coupled through their asymptotic normalization constants C_{1l} and C_{2l} . This coupling arises as follows. The ψ_{1l} and ψ_{2l} are single-channel wavefunctions which reproduce the real part of the phase shifts, but in order to establish their connection with the complex wavefunctions describing multichannel processes it is necessary to invent a fictitious outgoing scattering channel which permits the determination of an equivalence.

The wavefunctions ψ_{1l} and ψ_{2l} may be renormalized to yield functions ϕ_{1l} and ϕ_{2l} which satisfy equations (9) and have the asymptotic forms

$$\phi_{1l} \rightarrow \sin(k_1 r - \frac{1}{2}l\pi + \alpha_{1l}), \quad \phi_{2l} \rightarrow \sin(k_2 r - \frac{1}{2}l\pi + \alpha_{2l}). \quad (11)$$

This renormalization is carried out only to simplify subsequent equations, and does not affect the conclusions.

III. EQUIVALENT OPTICAL MODEL

The problem is to find for given α_{1l} , α_{2l} , and η the complex potential in equation (1) which yields the same \mathbf{T} matrix as the equivalent pseudo-scattering wavefunctions ϕ_{1l} and ϕ_{2l} (the \mathbf{T} matrix is the measurable quantity). This can be done as follows.

The inverse reaction calculation (Cook 1970, 1972) is used to determine effective potentials \bar{V}_1 and \bar{V}_2 such that wavefunctions $\bar{\phi}_1$ $\bar{\phi}_2$ satisfy the transposed energy equations

$$\frac{d^2 \bar{\phi}_{1l}}{dr^2} + \left(k_2^2 - \bar{V}_{1l} - \frac{l(l+1)}{r^2} \right) \bar{\phi}_{1l} = 0, \quad \frac{d^2 \bar{\phi}_{2l}}{dr^2} + \left(k_1^2 - \bar{V}_{2l} - \frac{l(l+1)}{r^2} \right) \bar{\phi}_{2l} = 0, \quad (12)$$

with the asymptotic forms

$$\bar{\phi}_{1l} \xrightarrow{(r \rightarrow \infty)} \sin(k_2 r - \frac{1}{2}l\pi + \alpha_{1l}), \quad \bar{\phi}_{2l} \xrightarrow{(r \rightarrow \infty)} \sin(k_1 r - \frac{1}{2}l\pi + \alpha_{2l}). \quad (13)$$

We now introduce complex asymptotic normalization constants A_{1l} , A_{2l} , B_{1l} , and B_{2l} such that for large r

$$A_{1l} \phi_{1l} + B_{1l} \bar{\phi}_{2l} \rightarrow \sin(k_1 r - \frac{1}{2}l\pi + \delta_{1l}), \quad A_{2l} \phi_{2l} + B_{2l} \bar{\phi}_{1l} \rightarrow \sin(k_2 r - \frac{1}{2}l\pi + \delta_{2l}),$$

where δ_{1l} and δ_{2l} are the complex phase shifts in channels 1 and 2 respectively. Hence we find

$$\left. \begin{aligned} A_{1l} &= \frac{\sin(\delta_{1l} - \alpha_{2l})}{\sin(\alpha_{1l} - \alpha_{2l})}, & A_{2l} &= \frac{\sin(\delta_{2l} - \alpha_{1l})}{\sin(\alpha_{2l} - \alpha_{1l})}, \\ B_{1l} &= \frac{\sin(\delta_{1l} - \alpha_{1l})}{\sin(\alpha_{1l} - \alpha_{2l})} = -\frac{i \sinh \beta_{1l}}{\sin(\alpha_{1l} - \alpha_{2l})}, & B_{2l} &= -\frac{i \sinh \beta_{2l}}{\sin(\alpha_{2l} - \alpha_{1l})}. \end{aligned} \right\} \quad (14)$$

The functions U_{1l} and U_{2l} defined as

$$U_{1l} = A_{1l} \phi_{1l}(k_1 r) + B_{1l} \bar{\phi}_{2l}(k_1 r), \quad U_{2l} = B_{2l} \bar{\phi}_{1l}(k_2 r) + A_{2l} \phi_{2l}(k_2 r) \quad (15)$$

will satisfy equation (1) provided

$$v_1 = \frac{A_1 V_1 \phi_1 + B_1 \bar{V}_2 \bar{\phi}_2}{A_1 \phi_1 + B_1 \bar{\phi}_2}, \quad v_2 = \frac{B_2 \bar{V}_1 \bar{\phi}_1 + A_2 V_2 \phi_2}{B_2 \bar{\phi}_1 + A_2 \phi_2} \quad (16)$$

are the complex potentials in each channel. Since the real pseudo-scattering wavefunctions and real potentials have been determined, we need to know the constants A_1 , A_2 , B_1 , and B_2 to find the complex potentials. More generally, one could use source terms, as occur in meson theory, of

$$V_c \phi_{lc} = \rho_c, \quad v_c U_{lc} = \xi_c \quad (17)$$

and the multichannel equations given by the asymptotic conditions (13) and (2). Whatever approach is used, the forms (11) and (13) lead to the results

$$\exp(i\delta_{cl}) = A_c \exp(i\alpha_{cl}) + \sum_{c' \neq c} B_{cc'} \exp(i\alpha_{c'l}), \quad (18a)$$

$$\exp(-i\delta_{cl}) = A_c \exp(-i\alpha_{cl}) + \sum_{c' \neq c} B_{cc'} \exp(-i\alpha_{c'l}). \quad (18b)$$

Since $\delta_{cl} = \alpha_{cl} + i\beta_{cl}$ as in equation (2), all quantities are known in equations (18)

except the constants A_c and B_{cc} . We shall now consider the determination of these quantities. Equations (18) state the connection between asymptotic normalization constants (C_{1l} and C_{2l}) which as functions of A_{1l} , A_{2l} , B_{1l} , and B_{2l} are no longer independent.

It is at this stage that we are confronted with the lack of uniqueness of the potential that is to be calculated. The arguments are quite general to this point, and upon close examination of equations (18) it is found that for an $n \times n$ collision matrix these equations consist of $2n$ equations containing $2n^2$ unknowns. Enforcing the requirement that the matrix B_{cc} should be symmetric, reduces the number of unknowns to $n^2 + n$. Even so, the elementary 2×2 case still cannot be solved uniquely for it has four equations and six unknowns. This is a serious deficiency of inverse reaction calculations.

IV. EXAMPLE OF COMPOUND NUCLEUS MODEL

As an illustration of a simple and experimentally verified model which allows one to overcome lack of other experimental data, let us suppose that a particular particle and target are observed to have two channels, a scattering channel and a distinct reaction channel. In the S matrix specifying this process, given by equations (4), the element S_{22} and the phase of S_{12} are arbitrary, and only δ_{1l} is known. To determine the unknowns, we introduce the equiphase assumption discussed by Cook (1967) to the reduced transition matrix in equation (8). This condition states that all phases of T' are equal. It yields the constraints

$$\tan 2\phi_l = -\eta \sin 2\alpha'_{1l} / (1 - \eta \cos 2\alpha'_{1l}), \quad \phi_l = \frac{1}{2}(\alpha'_{1l} + \alpha'_{2l}).$$

These can be found by equating the phases of elements in equation (8). The above procedure allows S_{22} and the phase of S_{12} to be found. This assumption has a basis in reality in that it represents the Bohr (1936) compound nucleus condition for the resonant part of the reaction. This condition is still of practical importance in nuclear theory.

V. CONCLUSIONS

The above method for calculating optical potentials in multichannel problems where only the complex scattering phase shifts are known has been seen to give both the complex potential required to reproduce the phase shift and an optical model wavefunction. Although such functions reproduce all the data, they are not of course unique. This difficult question of uniqueness is worthy of further investigation. We would point out, however, that the calculation of a set of consistent values of ρ_c has been performed successfully (Clayton 1972a, 1972b) for a wide range of phase shifts, and given this information the above method cannot fail to reproduce the data.

VI. REFERENCES

- BOHR, N. (1936).—*Nature* **137**, 344.
 CLAYTON, E. (1972a).—AAEC Rep. No. TM604.
 CLAYTON, E. (1972b).—M.Sc. Thesis, University of New South Wales.
 COOK, J. L. (1967).—*Aust. J. Phys.* **20**, 355.
 COOK, J. L. (1970).—AAEC Rep. No. TM560.
 COOK, J. L. (1972).—*Aust. J. Phys.* **25**, 167.
 LANE, A. M., and THOMAS, R. G. (1958).—*Rev. mod. Phys.* **30**, 257.
 PRESTON, M. A. (1962).—"Physics of the Nucleus." (Addison-Wesley: Massachusetts.)

