# A NOTE ON INVERSE SCATTERING CALCULATIONS
## OF ENERGY–INDEPENDENT POTENTIALS

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*Abstract*

It is shown that a method proposed for determining one single-channel potential from a real scattering phase shift using resonance parameters allows the determination of an energy-independent potential.

The non-uniqueness of single-channel potentials is now well established both analytically (Bargmann 1949*a*, 1949*b*; Clayton 1972) and numerically (Sabatier 1966*a*, 1966*b*, 1967; Sabatier and Quyen Van Phu 1971; Clayton 1972) for both energy-dependent and energy-independent forms. Therefore, given a set of data on a particular reaction there is no such thing as a "physical" potential but rather a class of such potentials, infinite in number and varying in shape, which reproduce a given set of phase shifts. This is true for any number of channels regardless of whether the potentials are dependent or independent of energy. Once this situation is recognized, it becomes clear that in quantum mechanics a potential is merely a device for reproducing data and the criterion for selecting one member of an infinite class is a matter of individual choice. We should try therefore to select a *definition* of a potential which possesses the least number of hypotheses. One such definition, which would be applicable if resonance parameters have been obtained from experiment, was proposed by Cook (1972), namely that the resonance reduced widths should be related to the free-particle reduced widths by a bilinear transformation. This hypothesis was sufficient to define a potential uniquely, but yielded an energy-dependent potential. In this note, an alternative method which gives an energy-independent potential is considered.

Using the notation of the previous paper (Cook 1972; hereinafter referred to as Paper I), we expand the wavefunction $U_l$ into an orthonormal set of states $U_\lambda(r)$ such that in each eigenstate of $l$ (omitting the $l$ suffix)

$$U(E,r) = \sum_\lambda A_\lambda(E) U_\lambda(r), \tag{1a}$$

and the $U_\lambda(r)$ into free-particle states $W_\mu(r)$,

$$U_\lambda(r) = \sum_\mu B_{\lambda\mu} W_\mu(r), \tag{1b}$$

such that the potential is

$$\mathscr{V}(E,r) = \sum_{\lambda\mu} A_\lambda(E) V_{\lambda\mu} W_\mu(r) \bigg/ \sum_{\lambda\mu} A_\lambda(E) B_{\lambda\mu} W_\mu(r), \tag{2}$$

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where $2mE = k^2$, $m$ being the reduced mass of the two-particle system, and

$$V_{\lambda\mu} = (E_\lambda - \mathscr{E}_\mu)B_{\lambda\mu} \tag{3}$$

with $E_\lambda$ and $\mathscr{E}_\mu$ the eigenvalues of energy corresponding to $U_\lambda(r)$, and $W_\mu(r)$ respectively. As in Paper I, we define

$$V_\lambda(r)\,U_\lambda(r) = \sum_\mu V_{\lambda\mu}\,W_\mu(r) \qquad \text{with} \qquad V_\lambda(r) \equiv \mathscr{V}(E_\lambda, r) \tag{4}$$

and a matrix of constants

$$Z_{\lambda\mu} = \int_0^a V_\lambda(r)\,U_\lambda(r)\,U_\mu(r)\,\mathrm{d}r. \tag{5}$$

We see from equations (3) and (4) that $\mathscr{V}(E, r)$ will be independent of energy provided that

$$V_\lambda(r) = \mathscr{V}(r) \qquad \text{for all } \lambda. \tag{6}$$

Equations (2) and (4) then yield

$$\mathscr{V}(r)\,U = \sum_\lambda A_\lambda(E)\,V_\lambda(r)\,U_\lambda(r) = \sum_{\lambda\nu} A_\lambda(E)\,Z_{\lambda\nu}\,U_\nu(r), \tag{7}$$

and so by equating coefficients of the energy-dependent terms $A_\lambda(E)$ we get

$$\sum_\nu Z_{\lambda\nu}\,U_\nu(r) = V_\lambda(r)\,U_\lambda(r) = \mathscr{V}(r)\,U_\lambda(r), \tag{8}$$

or in matrix notation

$$\mathbf{Z}\,U(r) = V_\lambda(r)\,U(r) = \mathscr{V}(r)\,U(r), \tag{9}$$

from which it follows that $\mathscr{V}(r)$ is an eigenvalue of the infinite matrix $\mathbf{Z}$ which has an eigenvector $U(r)$. However, $\mathbf{Z}$ is a constant matrix. In practical calculations we must always consider only a finite number of poles at each $E = E_\lambda$ in the reaction matrix, and therefore a finite number of $\lambda$'s. This proves to be an excellent approximation when reproducing phase shifts (Clayton 1972). It follows that $\mathbf{Z}$ has to be a finite matrix as well and therefore that it must have constant eigenvalues. We are now faced with the problem of how to overcome this apparent discrepancy with Paper I, in which equation (9) cannot hold unless $V_\lambda(r) = \mathscr{V}(r) = \text{const}$. It can be shown from equations (2) and (7) that

$$\mathbf{Z} = \mathbf{V}\,\mathbf{B}^t \qquad (\mathbf{V} \equiv V_{\lambda\mu}), \tag{10}$$

where $\mathbf{B}^t$ denotes the transpose of matrix $\mathbf{B}$. Specification of $\mathbf{B}$ and $\mathbf{V}$ therefore determines $\mathbf{Z}$.

We define a set of mutually orthogonal constant eigenvectors $U_{\lambda(\sigma)}$ by evaluating the finite matrix $\mathbf{V}$ from equation (3) and letting $U_{\lambda\sigma}$ be the eigenvectors of the matrix $\mathbf{Z}$ derived from equation (10). Since the expected infinite number of poles and residues in the reaction matrix cannot be obtained from experiment, we seek an alternative equation to (9). This equation must suffice to yield an energy-independent potential and to permit its complete evaluation with a knowledge of only $M$ values of

$E_\lambda$ and $\gamma^2$. To this end we define $M$ simple functions $\phi_\sigma$ ($\sigma = 1, \ldots, M$) such that

$$\phi_\sigma = (r_{\sigma+1} - r_\sigma)^{-\frac{1}{2}} \quad \text{for} \quad r_{\sigma+1} \geqslant r \geqslant r_\sigma, \left.\begin{array}{c} \\ \end{array}\right\} \tag{11}$$
$$= 0 \qquad\qquad\qquad \text{otherwise,}$$

and the interval $0 \leqslant r \leqslant a$ has been divided into $M$, not necessarily equal, intervals. Such functions obey the relation

$$\int_0^a \phi_\sigma \phi_\nu \, dr = \delta_{\sigma\nu}. \tag{12}$$

Since they can be expanded in terms of the orthonormal set $W_\mu(r)$ as

$$\phi_\sigma = \sum_{\mu=1}^\infty W_{\sigma\mu} W_\mu(r), \tag{13}$$

substitution of this expansion into equation (12) gives

$$\sum_\mu W_{\sigma\mu} W_{\nu\mu} = \delta_{\sigma\nu}, \tag{14}$$

so that $\mathbf{W}$ is an orthogonal matrix. It also follows from equations (12) and (13) that

$$W_{\mu\sigma} = \int_0^a W_\mu(r) \phi_\sigma \, dr. \tag{15}$$

We can likewise use the definition for $B_{\lambda\mu}$ in Paper I and define

$$U_{\lambda\sigma} = \int_0^a U_\lambda(r) \phi_\sigma \, dr. \tag{16}$$

Multiplying equation (1b) by $\phi_\sigma$ and integrating over $0 \leqslant r \leqslant a$, we get

$$U_{\lambda\sigma} = \sum_\mu B_{\lambda\mu} W_{\mu\sigma}, \tag{17}$$

while the same operation on equation (8) yields

$$\sum Z_{\lambda\nu} U_{\nu\sigma} = \int_0^a V_\lambda(r) U_\lambda(r) \phi_\sigma \, dr. \tag{18}$$

Since $\mathbf{W}$ and $\mathbf{B}$ are both orthogonal matrices, $\mathbf{U}$ is also an orthogonal matrix. We now postulate that $\mathscr{V}(r)$ is a simple function, i.e.

$$\mathscr{V}(r) = \sum_{\rho=1} V_\rho \Theta(r_{\rho+1} - r) \Theta(r - r_\rho), \tag{19}$$

where $\Theta(x)$ is the Heaviside function. Equation (18) then yields

$$\sum_\nu Z_{\lambda\nu} U_{\nu\sigma} = V_\sigma U_{\lambda\sigma}. \tag{20}$$

Since $\mathbf{Z}$ is a finite constant matrix, equation (20) can be interpreted as the equation for the $M$ eigenvalues $V_\sigma$ of $\mathbf{Z}$ and eigenvectors $U_\sigma$. The method is therefore to define $\mathbf{Z}$ by equation (10) and evaluate its eigenvalues and eigenvectors. Substitution of the eigenvalues into equation (19) give us an energy-independent potential over the energy range considered.

In the above method we have only fitted to $M$ poles and the energy-independent eigenvectors $U_\lambda(r)$ cannot reproduce the continuous energy term in the Schrödinger equation for a finite sum because the relation

$$\sum_{\lambda=1}^{M} E_\lambda A_\lambda(E)\, U_\lambda(r) = E \sum_{\lambda=1}^{M} A_\lambda(E)\, U_\lambda(r) \qquad (21)$$

does not hold, for the well-known reason that the series as $M$ tends to infinity is not uniformly convergent and equation (21) is only possible in this limit. Therefore, we must somehow include the infinity of other poles determined by the simple potential (19). This is done by integrating the Schrödinger equation using (19) so that the infinities in the reaction matrix

$$R(E) = \Psi(E,a)/\{a\, \Psi'(E,a) - b\, \Psi(E,a)\} \qquad (22)$$

are at the positions of the infinite number of poles. In equation (22), $\Psi(E,a)$ is the total wavefunction at $r = a$, $a$ is the nuclear radius, and $b$ is the boundary condition parameter. The more poles one chooses to use, the closer $\mathscr{V}$ tends to a smooth function. However, since the choice of the $\mathbf{B}$ matrix remains arbitrary, the choice of $\mathbf{Z}$ and hence of $\mathscr{V}$ is also arbitrary, subject to the constraints mentioned above.

The observable $M$ poles in $R(E)$ have now all been taken into account with correct residues, but the potential (19) will probably not give the correct constant term in the fitted $R(E)$, representing the sum over distant poles. One can allow for this by splitting $R(E)$ into two contributions as

$$R(E) = \sum_{\lambda=1}^{M} \gamma_\lambda^2/(E_\lambda - E) + R_0, \qquad (23)$$

where

$$R_0 \approx \sum_{\lambda=M+1}^{\infty} \gamma_\lambda^2/(E_\lambda - E) \approx \text{const.}$$

and the first few residues outside the energy range considered are adjusted to give the correct $R_0$. This implies a deviation from the evaluated potential (19) in distant energy regions, but ensures that the correct phase shift is always obtained. Clayton (1972) gives a more detailed discussion of this point.

A final point is that it may seem strange that both an energy-dependent and energy-independent potential can be evaluated from the same $\mathbf{B}$ matrix. However, it should be recalled that the method in Paper I which yields a unique energy-dependent potential uses a $\mathscr{V}(r)$ that is always a continuous function of $r$ from 0 to $a$, while in the present paper $\mathscr{V}(r)$ is explicitly discontinuous in the above interval but is a simple function of $r$. The latter condition is sufficient to permit the calculation of an energy-independent $\mathscr{V}$ even though the same $\mathbf{B}$ is used in both cases.

## References

BARGMANN, V. (1949a).—*Phys. Rev.* **75**, 301.

BARGMANN, V. (1949b).—*Rev. mod. Phys.* **21**, 488.

CLAYTON, E. (1972).—M.Sc. Thesis, University of New South Wales.

COOK, J. L. (1972).—*Aust. J. Phys.* **25**, 167.

SABATIER, P. C. (1966a).—*J. math. Phys.* **7**, 1515.

SABATIER, P. C. (1966b).—*J. math. Phys.* **7**, 2079.

SABATIER, P. C. (1967).—*J. math. Phys.* **8**, 905.

SABATIER, P. C., and QUYEN VAN PHU, F. (1971).—*Phys. Rev.* D **4**, 127.