Optimization of Nuclear Resonance Reaction Calculations

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An important current problem is to find the most economical and physically significant method of calculating nuclear resonant cross sections. Tobocman and co-workers have discussed an R-matrix type of approach in which the wave function is restricted to be a linear combination of a given finite set of states associated with the resonances. That work presented several different formulas for calculation, leaving uncertainty as to which, if any, was the best one. This paper gives systematic reasons why one specific formula should be more accurate than all others. This result applies to any set of states, and is not restricted to the special set used in the previous work. A curious incidental result in this paper is that the variational principle for scattering problems introduced by Kohn fails to give a stationary result when applied to the present problem.

I. INTRODUCTION

IN a stimulating set of papers, Tobocman and co-workers[1–3] have discussed the problem of calculating resonant cross sections. Generally, in this problem one assumes a given set of states, which ultimately give rise to the resonances, and enquires what is the best (i.e., most accurate) form of the scattering matrix that can be obtained from these states. In practice these states are shell-model states. One would like to use harmonic-oscillator states because of their simplicity, but this is prohibited in most treatments because such states vanish at infinity. Tobocman and co-workers have avoided this difficulty by using the methods of R-matrix theory. Since the R matrix is calculated from the finite "internal" region of space then oscillator states can give meaningful results.

It remains to specify the precise formula that should be used for calculating the collision matrix. This is not a trivial problem. When the given basis is complete, there are different ways of writing the exact collision matrix in terms of the basis states. Provided the basis is complete, all such ways are equivalent and correct, but this is no longer true when a finite (i.e., incomplete) basis is used. One must then decide which way is the best (i.e., most accurate).

A warning that some choices can be very poor follows from a simple example. Suppose that, in a one-body problem, we have a complete set of states satisfying a homogeneous boundary condition at a radius just outside the surface radius of the internal region. Both the wave function and its derivative can, in principle, be expanded in terms of this set inside the internal region and on its surface. However, if we start with a finite set and add more and more states, the approach to the exact derivative is slower than that of the exact function (because the derivative fails to converge at the boundary radius). Thus any formula for the collision matrix involving the expansion of the derivative should be avoided.

Tobocman and co-workers have considered the special case when the basis states are those defined inside a boundary larger than the surface of the interior region. They present several different formulas for the collision matrix. In the present paper arguments are given for a unique best formula for the collision matrix. This formula applies not only to the special states used in previous work, but to any set of states.

In Secs. II and III we describe an attempt to find a best formula by use of a stationary principle for scattering which is closely related to that of Kohn.[4] In Secs. IV and V alternative arguments leading to the same formula are given. In Sec. VI, the discussion is specialized to the particular states used by Tobocman and co-workers, and further arguments, specific to this class of states, are given in favor of the suggested best formula.

A curious incidental result is that the stationary principle fails to give a stationary result in the present context when the trial functions have the form of linear combinations of a fixed number of states. Nevertheless, the principle gives a unique formula which may be regarded as the best one because of its derivation from the alternative treatments.

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[1] W. Tobocman and M. A. Nagarajan, Phys. Rev. **138**, 1351 (1965).

[2] M. A. Nagarajan, S. K. Shah, and W. Tobocman, Phys. Rev. **140**, 63 (1965).

[3] J. E. Purcell, Case Western Reserve University, Physics Department Technical Report (unpublished).

[4] W. Kohn, Phys. Rev. **74**, 1763 (1948).

II. STATIONARY PRINCIPLE FOR SCATTERING PROBLEMS

Kohn[4] has given a stationary principle for one-body scattering, suitable for the case when the trial functions are defined only in the interaction region, i.e., the internal region bounded by $r=a$ (say). The variation functional is

$$L(\psi_t)=[\psi_t(a)]^{-2}\left(\frac{\hbar^2}{2m}[(r\psi_t)(r\psi_t)']_{r=a}+\int_0^a dr\, r^2\psi_t(H-E)\psi_t\right), \quad (2.1)$$

where the prime denotes radial differentiation and where the angular part of the trial function has been suppressed for simplicity. Kohn shows that this functional is stationary for general variations around the exact solution of $(H-E)\,\psi=0$,

$$L(\psi_t)-L(\psi)=\text{second order in } (\psi_t-\psi),$$

and the stationary value of $L(\psi_t)$ is

$$L(\psi)=(\hbar^2a^2/2m)f, \quad (2.2)$$

wherein f is the logarithmic derivative,

$$f=[(r\psi)'(r\psi)^{-1}]_{r=a}. \quad (2.3)$$

Using the form of ψ valid for $r\geq a$,

$$r\psi=I-UO, \quad (2.4)$$

where U is the collision function, and I and O are incoming and outgoing waves:

$$I\underset{r\to\infty}{\sim}\exp(-ikr), \qquad O\underset{r\to\infty}{\sim}\exp(+ikr). \quad (2.5)$$

The well-known relation between f and U is easily derived:

$$U=[(fI-I')(fO-O')^{-1}]_{r=a}. \quad (2.6)$$

Thus $L(\psi_t)$ provides a stationary principle for the collision function.

The functional $L(\psi_t)$ has the disadvantage that its quotient form makes it difficult to generalize it to the many-channel case. However, it is easy to find another functional, equivalent to the above, but which can be generalized:

$$M(\psi_t)\equiv(\hbar^2/2m)\{(r\psi_t)[(r\psi_t)'-O^{-1}O'(r\psi_t)] -2(r\psi_t)[(r\psi)'-O^{-1}O'(r\psi)]\}_{r=a}+\int_0^a dr\, r^2\psi_t(H-E)\psi_t. \quad (2.7)$$

This functional has the same basic properties as $L(\psi_t)$: It is an explicit function of ψ_t; it is stationary about $\psi_t=\psi$; and its stationary value gives the collision matrix. Further, it can be generalized to the many-channel case. These properties will now be demonstrated.

The presence of the (unknown) function ψ in $M(\psi_t)$ does not conflict with M being an explicit function of ψ_t, because ψ occurs in a combination that only depends on the known ingoing-wave part of ψ:

$$[(r\psi)'-O^{-1}O'(r\psi)]_{r=a}=[I'-O^{-1}O'I]_{r=a}=-2ik/O(a). \quad (2.8)$$

The stationary property of $M(\psi_t)$ can be checked directly from the above form. Alternatively, we may first rewrite $M(\psi_t)$:

$$M(\psi_t)=F(\psi_t,\psi_t)-F(\psi,\psi_t)-F(\psi_t,\psi), \quad (2.9)$$

where

$$F(\phi,\chi)\equiv(\hbar^2/2m)[(r\phi)(r\chi)'-O^{-1}O'(r\chi)]_{r=a}+\int_0^a dr\, r^2\phi(H-E)\chi. \quad (2.10)$$

By using the facts that $(H-E)\psi=0$ and

$$\int_0^a dr\, r^2(\psi H\psi_t-\psi_t H\psi)=(\hbar^2/2m)[(r\psi)'(r\psi_t)-(r\psi)(r\psi_t)']_{r=a},$$

it directly follows from this form of M that

$$M(\psi_t)-M(\psi)=F(\psi_t-\psi,\psi_t-\psi)=\text{second order in } (\psi_t-\psi), \quad (2.11)$$

so that M is stationary about $\psi_t=\psi$.

Finally, the stationary value of M is

$$M(\psi)=-(\hbar^2/2m)\{(r\psi)[(r\psi)'-O^{-1}O'(r\psi)]\}_{r=a} =2ik\hbar^2[I(a)-UO(a)]/2mO(a), \quad (2.12)$$

which determines the collision function U.

The extension of the principle to the multichannel case can be done most simply by switching to the Bloch $\mathfrak{L}$-operator formalism.[5] On defining the operator

$$\mathfrak{L}(b)=(\hbar^2/2mr)\delta(r-a)[(d/dr)r-b], \quad (2.13)$$

and writing the operator for the particular choice $b=aO'O^{-1}$ simply as $\mathfrak{L}$ (i.e., without argument), we can rewrite F as

$$F(\phi,\chi)=\langle\phi^\dagger\mid H+\mathfrak{L}-E\mid\chi\rangle, \quad (2.14)$$

in which angular wave functions are now included. The dagger on $\phi^\dagger$ denotes the complex conjugate of the time-reversed state:

$$\langle\mathbf{r}\mid\phi^\dagger\rangle=\langle\mathbf{r}\mid K\mid\phi\rangle^*,$$

i.e., $\phi^\dagger$ involves the same angular part as ϕ, but the complex conjugate of the radial part.

The multichannel version of $\mathfrak{L}(b)$ is

$$\mathfrak{L}(b)=\sum_c\mid c)(\hbar^2/2m_cr_c)\delta(r_c-a_c)[(d/dr_c)r_c-b_c](c\mid, \quad (2.15)$$

[5] A. M. Lane and D. Robson, Phys. Rev. **151**, 774 (1966).

where b represents the set of numbers b_c and $|\,c)$ is the channel wave function of channel c, i.e., the product of the internal and relative angular wave functions for the two particles.

It follows just as before that $M(\psi_t)$ defined by (2.9) in terms of F given by (2.14) is stationary in the sense expressed by (2.11). If α_c are the amplitudes of incoming waves,

$$\vartheta_c = r_c^{-1} I_c(r_c)\,|\,c)$$

in ψ, then ψ has the asymptotic forms

$$\psi \underset{r_c\to\infty}{\sim} \alpha_c \vartheta_c - \sum_{c'} \alpha_{c'} U_{cc'} \mathcal{O}_c (v_c v_{c'}^{-1})^{1/2}, \tag{2.16}$$

in which v_c are channel velocities, $\mathcal{O}_c$ are outgoing waves,

$$\mathcal{O}_c = r_c^{-1} O_c(r_c)\,|\,c),$$

and $U_{cc'}$ are elements of the collision matrix.

The many-channel $M(\psi_t)$ given by (2.9), (2.14), and (2.16) is an explicit function of ψ_t, provided that $H+\mathfrak{L}$ has the Hermiticity property

$$\langle \psi^\dagger \,|\, H+\mathfrak{L} \,|\, \psi_t\rangle = \langle \psi_t{}^\dagger \,|\, H+\mathfrak{L} \,|\, \psi\rangle, \tag{2.17}$$

which is valid if ψ contains no open three-body channels and the sum over c in $\mathfrak{L}$ includes all two-body channels. Given (2.17), and using $(H-E)\psi=0$, the dependence of $M(\psi_t)$ on ψ can be put in the form $\mathfrak{L}\,|\,\psi\rangle$. If the α_c are given this is known.

The exact stationary value of $M(\psi_t)$ is

$$M(\psi) = -\sum_c (\hbar^2/2m_c) \times \{[\alpha_c I_c - \sum_{c'} U_{cc'} \alpha_{c'} O_c (v_c v_{c'}^{-1})^{1/2}] \times [\alpha_c (I_c' - (O_c'/O_c) I_c)]\}_{r_c = a_c}. \tag{2.18}$$

The stationary value from the practical use of the principle will be quadratic in the α_c also. Since these are independent variables, one can obtain the set of matrix elements $U_{cc'}$ by equating coefficients.

Practical Use of a Stationary Principle

The motive in using a variation principle, whether minimum or merely stationary, is to find the best value of the collision matrix by making use of the functional $M(\psi_t)$ which is stationary at that value for variations of ψ_t about the exact solution ψ. In practical cases, the set of trial functions ψ_t that is used will not, in general, include the exact solution ψ. The standard procedure in using a stationary (as opposed to minimum) principle is to *assume* that the function (ψ_{t0}, say) obtained as the stationary point of $M(\psi_t)$ for *restricted* variations gives a good value [viz., $M(\psi_{t0})$] for the exact stationary quantity $M(\psi)$. This is the only evident systematic procedure for obtaining a best value. If the set ψ_t includes the most significant variations about ψ, it will be a sound set of trial functions. Even when this is not true and ψ_{t0} is not very close to ψ, then the value for $M(\psi_{t0})$ may still be good, since M is stationary at $\psi_t=\psi$. Unfortunately, there is no way of estimating the error. This is the basic weakness of a stationary principle as opposed to a minimum one where ψ_{t0} does definitely give the best (i.e., least) value for $M(\psi)$ obtainable amongst a restricted set ψ_t.

From this discussion, we will assume that the best value for $M(\psi_t)$ is obtained as $M(\psi_{t0})$, where ψ_{t0} is such that

$$M(\psi_t) - M(\psi_{t0}) = \text{second order in } (\psi_t - \psi_{t0}), \tag{2.19}$$

for variations in the restricted set of ψ_t. From the definitions (2.9) and (2.14), and the Hermiticity relation (2.17), if $\Delta\psi_t = \psi_t - \psi_{t0}$,

$$M(\psi_t) - M(\psi_{t0}) = \langle \Delta\psi_t{}^\dagger \,|\, A \,|\, \psi_{t0} - \psi\rangle + \langle \psi_{t0}{}^\dagger - \psi^\dagger \,|\, A \,|\, \Delta\psi_t\rangle + \langle \Delta\psi_t{}^\dagger \,|\, A \,|\, \Delta\psi_t\rangle, \tag{2.20}$$

where for brevity we have written

$$A = H + \mathfrak{L} - E. \tag{2.21}$$

The stationary condition is thus

$$\langle \Delta\psi_t{}^\dagger \,|\, A \,|\, \psi_{t0} - \psi\rangle + \langle \psi_{t0}{}^\dagger - \psi^\dagger \,|\, A \,|\, \Delta\psi_t\rangle = 0 \tag{2.22}$$

or

$$\langle \psi_t{}^\dagger \,|\, A \,|\, \psi_{t0} - \psi\rangle + \langle \psi_{t0}{}^\dagger - \psi^\dagger \,|\, A \,|\, \psi_t\rangle = \text{const } (C, \text{ say}), \tag{2.23}$$

for ψ_t near ψ_{t0}.

III. DERIVATION OF THE BEST FORMULA FOR U USING THE STATIONARY PRINCIPLE

When ψ_t is restricted to be a linear combination of a given set of functions

$$\psi_t = \sum_{n=1}^{M} d_n \phi_n, \tag{3.1}$$

then the stationary condition (2.23) gives, on varying the d_n one at a time,

$$\langle \phi_m{}^\dagger \,|\, A \,|\, \psi_{t0} - \psi\rangle + \langle \psi_{t0}{}^\dagger - \psi^\dagger \,|\, A \,|\, \phi_m\rangle = 0, \tag{3.2}$$

for all m. On inserting the form

$$\psi_{t0} = \sum_{n=1}^{M} d_{n0} \phi_n, \tag{3.3}$$

we get the solution

$$\mathbf{d} = (\mathbf{A} + \mathbf{A}^T)^{-1} \mathbf{g}, \tag{3.4}$$

where $\mathbf{g}$ is the column vector with elements

$$g_n = 2\langle \phi_n{}^\dagger \,|\, \mathfrak{L} \,|\, \psi\rangle \tag{3.5}$$

and $\mathbf{A}$ is a square matrix with elements

$$A_{mn} = \langle \phi_m{}^\dagger \,|\, A \,|\, \phi_n\rangle. \tag{3.6}$$

It is easily checked, from (2.9), (2.14), and (3.4), that the stationary value is

$$M(\psi_{t0}) = -\tfrac{1}{2} \mathbf{g}^{\dagger T} (\mathbf{A} + \mathbf{A}^T)^{-1} \mathbf{g}. \tag{3.7}$$

One-Body Case

In this case, g_n is simply related to the reduced-width amplitude γ_n:

$$g_n=2(\hbar^2a/2m)^{1/2}(I'-O^{-1}O'I)_{r=a}\gamma_n, \quad (3.8)$$

with

$$\gamma_n=(\hbar^2a/2m)^{1/2}\phi_n(a). \quad (3.9)$$

Using the exact stationary value (2.12), we find for the collision function

$$U=O^{-1}I+2ika[O(a)]^{-2}R, \quad (3.10)$$

where R is defined as

$$R=2\gamma^T(\mathbf{A}+\mathbf{A}^T)^{-1}\gamma. \quad (3.11)$$

Equation (3.10) has the form of the Kapur-Peierls collision function where the resonances arise from the R function defined in (3.11). Equations (3.10) and (3.11) represent the result in the one-body case, i.e., given a set of functions ϕ_n, the best form of the collision matrix is obtained by constructing the matrix $\mathbf{A}$ and vector γ from (3.6) and (3.8), then forming R via (3.11) and inserting this in (3.10).

A wide range of different, but equivalent, forms of U may be obtained by algebraic manipulations, using the fact that the matrix $\mathcal{L}_{mn}$ contained in $\mathbf{A}$ has the simple form of a sum of two products:

$$\mathcal{L}_{nm}=\langle\phi_n{}^\dagger\mid\mathcal{L}\mid\phi_m\rangle$$
$$=(\hbar^2/2m)\{(r\phi_n)[(r\phi_m)'-O^{-1}O'(r\phi_m)]\}_{r=a}. \quad (3.12)$$

The various forms of U are described in Appendix A. Using these forms, one can show that the form (3.10) for U differs from that obtained using (2.6) and an evaluation of the logarithmic derivative f by differentiating (3.3). In the special case when the ϕ_n satisfy the same fixed boundary condition at $r=a$, say $(r\phi_n)'/(r\phi_n)=b$, then f obtained from (3.3) equals the constant b, and so is an arbitrary value depending entirely on the basis chosen. Thus, in this case, one has a check on the assertion that (3.10) is superior to some other formulas for U.

General Many-Body Case

Formulas (3.1) to (3.6) apply to this case, but now (3.7) becomes [on using (2.16)]

$$g_n=\sum_c \alpha_c(\hbar^2a_c/2m_c)^{1/2}(I_c'-O_c^{-1}O_c'I_c)_{r_c=a_c}\gamma_{nc}, \quad (3.13)$$

wherein

$$\gamma_{nc}=(\hbar^2a_c/2m_c)^{1/2}\langle r_c^{-2}\delta(r_c-a_c)\,(c\mid\phi_n\rangle. \quad (3.14)$$

On equating the stationary value (3.7) to the exact form (2.18) and using (3.13) we obtain for the best calculated value of the collision matrix

$$U_{cc'}=(O_c^{-1}I_c)_{r_c=a_c}\delta_{cc'}+\frac{2i(k_ck_{c'}a_ca_{c'})^{1/2}}{O_c(a_c)O_{c'}(a_{c'})}R_{cc'}, \quad (3.15)$$

in which

$$R_{cc'}=2\gamma_{c'}{}^T(\mathbf{A}+\mathbf{A}^T)^{-1}\gamma_c. \quad (3.16)$$

This is the main result of the present work. It is a unique explicit formula for the collision matrix when the trial functions are linear combinations of a given set of function ϕ_n.

Failure Of Stationary Property

It is a remarkable fact that the stationary principle, described in Sec. II, actually ceases to be stationary when it is applied to trial functions which are linear combinations, as we have just done above. Since the application of the principle above appears to be quite straightforward, and leads to a unique result, without anything "blowing up", this fact is unexpected. In fact, in using this principle (2.1), Kohn[4] applied it to linear combinations without observing that it failed to be stationary. However, it is easy to demonstrate. From Eq. (3.2), it follows that the constant C in (2.23) vanishes, so that

$$\langle\psi_{t0}{}^\dagger\mid A\mid\psi_{t0}-\psi\rangle=0. \quad (3.17)$$

It then follows from the definition (2.9) and (2.14) of $M(\psi_t)$ that

$$M(\psi_{t0})-M(\psi)=\langle\psi_{t0}{}^\dagger-\psi^\dagger\mid A\mid\psi_{t0}-\psi\rangle$$
$$=\langle\psi^\dagger\mid A\mid\psi-\psi_{t0}\rangle$$
$$=\langle\psi^\dagger-\psi_{t0}{}^\dagger\mid\mathcal{L}\mid\psi\rangle. \quad (3.18)$$

The last line is explicitly first order in $(\psi_{t0}-\psi)$ [because it contains $(\psi_{t0}-\psi)$ evaluated at the surface so that no integral cancellation can occur]. Thus, the *apparent* second-order quantity $\langle\psi_{t0}{}^\dagger-\psi^\dagger\mid A\mid\psi_{t0}-\psi\rangle$ is actually first order. The only evident explanation of this paradox is that the surface derivative in the matrix element, which appears with a δ function and so contributes finitely, is not first order but zero order. That this is the correct interpretation is strongly suggested by the special case when all ϕ_n satisfy a fixed boundary condition $(r\phi_n)'(r\phi_n)^{-1}=b/a$ at $r=a$; in this case $(r\psi_{t0})'-(r\psi)'$ is trivially of zero order, since

$$(r\psi_{t0})'(r\psi_{t0})^{-1}=b/a.$$

Another special feature of the case of linear combinations is as follows. Keeping to the one-body case for simplicity, $M(\psi_t)$ gives a stationary principle for $\psi(a)$ as is evident from (2.12) with (2.4). The "stationary" value $M(\psi_{t0})$ for the case of linear combinations is of exactly the same form:

$$M(\psi_{t0})=(\hbar^2a/2m)[2ik/O(a)]\psi_{t0}(a) \quad (3.19)$$

[see (3.7) and (3.3) with (3.4)]. It should be stressed that the failure of the stationary condition is specific to linear combinations. Neither (3.17) nor (3.19) is valid for general trial functions.

The fact that a stationary principle can fail to be stationary when used with a particular class of trial functions is not usually mentioned in standard texts on quantum mechanics, but is discussed in more specialized and mathematical texts. The failure of the stationary property means, of course, that we must be more cautious in claiming merit for the result (3.10) [or (3.15)].

The question which remains is whether this result has any claim to be "best" in view of the failure of the stationary property. We contend that it does. The mere fact that the principle yields a unique result suggests that there is something special about it. In Secs. IV and V below, essentially the same result is derived via other methods. In Sec. VI further arguments are given for the particular class of functions ϕ_n used by Tobocman and co-workers.

IV. DERIVATION OF THE BEST FORMULA BY TRUNCATING THE SOLUTION OF THE DYNAMICAL EQUATION

The exact dynamical equation for the wave function is[5]

$$(H+\mathfrak{L}-E)\,|\,\psi\rangle=\mathfrak{L}\,|\,\psi\rangle$$
$$=\mathfrak{L}\,|\,\sum_c \alpha_c \mathcal{G}_c\rangle. \qquad (4.1)$$

If the states ϕ_n $(n=1, 2,\cdots)$ form a complete set, then an equivalent statement is

$$\langle\phi_n{}^\dagger\,|\,H+\mathfrak{L}-E\,|\,\psi\rangle=\langle\phi_n{}^\dagger\,|\,\mathfrak{L}\,|\,\psi\rangle, \qquad (4.2)$$

for all n. On expanding ψ in terms of the ϕ_n,

$$\psi=\sum_{n=1}^{\infty} d_n\phi_n, \qquad (4.3)$$

and inserting this in (4.2) gives:

$$\mathbf{Ad}=\tfrac{1}{2}\mathbf{g},$$

so that

$$\mathbf{d}=\tfrac{1}{2}\mathbf{A}^{-1}\mathbf{g}, \qquad (4.4)$$

which is quite similar to, but not quite the same as, the stationary-principle result (3.4). The two forms are identical if $\mathbf{A}$ is symmetrical, i.e., if $H+\mathfrak{L}$ is Hermitian in the sense (2.17) for the basis ϕ_n. Actually, the left-hand side of (4.2) can be reversed, $\phi_n{}^\dagger\rightarrow\psi^\dagger$, $\psi\rightarrow\phi_n$, because of (2.17), and this leads to (4.4) with $\mathbf{A}^T$ in place of $\mathbf{A}$. Clearly (4.4) can be replaced by

$$\mathbf{d}=\tfrac{1}{2}[\alpha\mathbf{A}+(1-\alpha)\mathbf{A}^T]^{-1}\mathbf{g}, \qquad (4.5)$$

where the right-hand side must be the same for all α.

In practice, the given set of states ϕ_n is finite (i.e., incomplete), say $n=1,\cdots, M$. On restricting n in (4.2) and (4.3), we get an approximate solution of the form (4.5) where the dimensions of $\mathbf{A}$, $\mathbf{d}$, $\mathbf{g}$ are $M\times M$, $1\times M$, and $1\times M$, respectively. This approximate solution will depend on α unless $\mathbf{A}$ is symmetric, i.e., unless $(H+\mathfrak{L})$ is Hermitian in the set ϕ_n. This will be so in practical calculations, usually exactly, since it requires only that the set ϕ_n should be expressible in terms of two-body break-up channels only. (This is trivially valid for the one-body case). Thus, for practical purposes, the present derivation gives the same collision function as the one found from the stationary principle, viz., (3.15).

V. DERIVATION OF THE BEST FORMULA BY USE OF AN EFFECTIVE UNIT OPERATOR

The derivation in the last section may be rephrased by introducing the truncation of the set ϕ_n in the form of an effective unit operator.

The collision matrix U is expressible[5] in terms of matrix elements of $\mathcal{G}\equiv A^{-1}$ taken between known states. Thus the problem of giving an explicit form of $\mathbf{U}$ in terms of a given complete set ϕ_n $(n=1, 2,\cdots, \infty)$ will be solved once we have a unit operator in terms of the ϕ_n, say,

$$1=\sum_n\sum_m |\,\phi_n\rangle N_{nm}{}^\infty\langle\phi_m{}^\dagger\,|$$
$$=|\,\boldsymbol{\phi}\rangle\mathbf{N}^\infty\langle\boldsymbol{\phi}^\dagger\,| \quad \text{(say)}, \qquad (5.1)$$

since then,

$$\mathcal{G}=1\times\mathcal{G}\times 1=\sum_{n,m,n',m'} |\,\phi_n\rangle N_{nm}{}^\infty\mathcal{G}_{mm'}N_{m'n'}{}^\infty\langle\phi_{n'}{}^\dagger\,|$$
$$=|\,\boldsymbol{\phi}\rangle\mathbf{N}^\infty\mathbf{G}\mathbf{N}^\infty\langle\boldsymbol{\phi}^\dagger\,|\,, \qquad (5.2)$$

where $\mathbf{G}$ is the matrix $[\mathcal{G}_{mm'}]$.

In practice, the given set of states ϕ_n is finite (i.e., incomplete), so we wish to form an approximate (effective) unit operator for this case. To do this, we first shows that the exact unit operator may be given the form

$$1=\sum_{n,m=1}^{M} |\,\phi_n\rangle N_{nm}\langle\phi_m{}^\dagger\,| + \sum_{l,k=M+1}^{\infty} |\,\phi_l\rangle X_{lk}\langle\phi_k{}^\dagger\,|$$
$$=|\,\boldsymbol{\phi}\rangle_M\mathbf{N}\langle\boldsymbol{\phi}^\dagger\,|_M+|\,\boldsymbol{\phi}\rangle_r\mathbf{X}\langle\boldsymbol{\phi}^\dagger\,|_r, \qquad (5.3)$$

in which $|\,\boldsymbol{\phi}\rangle_M$ is a row vector $|\,\phi_1\rangle\,|\,\phi_2\rangle\cdots|\,\phi_M\rangle$, and $|\,\boldsymbol{\phi}\rangle_r$ (r=remainder) is the row vector $|\,\phi_{M+1}\rangle\,|\,\phi_{M+2}\rangle\cdots|\,\phi_\infty\rangle$. We fix $\mathbf{N}$ by the condition that the first term is the exact unit operator within the subspace of terms $n=1, 2,\cdots, M$. That this choice is possible and consistent is checked by the fact that it leads to a solution for both $\mathbf{N}$ and $\mathbf{X}$ as we shall now show.

Writing $\mathbf{O}_{Mr}$ for the matrix $\langle\phi_m{}^\dagger\,|\,\phi_l\rangle$ with m in $1,\cdots, M$ and l in $M+1,\cdots,\infty$, and similarly for $\mathbf{O}_{rM}$, $\mathbf{O}_{MM}$, $\mathbf{O}_{rr}$, we have

$$\mathbf{O}_{MM}=\mathbf{O}_{MM}\mathbf{N}\mathbf{O}_{MM},$$
$$\mathbf{O}_{Mr}\mathbf{X}\mathbf{O}_{rM}=0.$$

From the first relation it follows that

$$\mathbf{N}=\mathbf{O}_{MM}{}^{-1}. \qquad (5.4)$$

To solve for $\mathbf{X}$, we form other matrices $\mathbf{O}_{rM}$, etc., with the unit operator and get

$$\mathbf{O}_{rM}=\mathbf{O}_{rM}\mathbf{N}\mathbf{O}_{MM}+\mathbf{O}_{rr}\mathbf{X}\mathbf{O}_{rM},$$

whence

$$\mathbf{O}_{rr}\mathbf{X}\mathbf{O}_{rM}=0,$$

and similarly

$$\mathbf{O}_{Mr}\mathbf{X}\mathbf{O}_{rr}=0.$$

Finally,

$$\mathbf{O}_{rr}=\mathbf{O}_{rM}\mathbf{N}\mathbf{O}_{Mr}+\mathbf{O}_{rr}\mathbf{X}\mathbf{O}_{rr}.$$

Provided that $\mathbf{O}_{rr}^{-1}$ exists, a unique solution for $\mathbf{X}$ exists, i.e.,

$$\mathbf{X}=\mathbf{O}_{rr}^{-1}-\mathbf{O}_{rr}^{-1}\mathbf{O}_{rM}\mathbf{N}\mathbf{O}_{Mr}\mathbf{O}_{rr}^{-1}. \tag{5.5}$$

Even if $\mathbf{O}_{rr}^{-1}$ does not exist at least one solution for $\mathbf{X}$ can easily be found (Appendix B). [Note that we also have

$$\mathbf{X}\mathbf{O}_{rM}=\mathbf{O}_{Mr}\mathbf{X},$$

which when combined with (5.5) yields a relation involving the $\mathbf{O}$ matrices only:

$$\mathbf{O}_{rM}=\mathbf{O}_{rM}\mathbf{N}\mathbf{O}_{Mr}\mathbf{O}_{rr}^{-1}\mathbf{O}_{rM}. \tag{5.6}$$

As shown in Appendix II, all these relations are consistent with the properties of $\mathbf{O}$ provided $\mathbf{O}^2=\mathbf{O}$, which is the property consistent on completeness of the ϕ_n for $n=1,\cdots,\infty$]. Thus the form (5.3) of the unit operator is permissible; further, the choice $\mathbf{N}=\mathbf{O}_{MM}^{-1}$ is unique since it makes the first term in (5.3) the exact unit operator in the subspace $\phi_1,\cdots,\phi_M$.

Using the unit operator (5.3), $\mathcal{G}$ has the form

$$\mathcal{G}=|\,\boldsymbol{\phi}\rangle_M\mathbf{N}\mathbf{G}\mathbf{N}\langle\boldsymbol{\phi}^\dagger\,|_M+|\,\boldsymbol{\phi}\rangle_M\mathbf{N}\mathbf{G}\mathbf{X}\langle\boldsymbol{\phi}^\dagger\,|_r + |\,\boldsymbol{\phi}\rangle_r\mathbf{X}\mathbf{G}\mathbf{N}\langle\boldsymbol{\phi}^\dagger\,|_M+|\boldsymbol{\phi}\rangle_r\mathbf{X}\mathbf{G}\mathbf{X}\langle\boldsymbol{\phi}^\dagger\,|_r. \tag{5.7}$$

Inserting the unit operator in $\mathcal{G}A=1$ yields

$$(\mathbf{N}\mathbf{G}\mathbf{N})\mathbf{A}_{MM}+(\mathbf{N}\mathbf{G}\mathbf{X})\mathbf{A}_{rM}=\mathbf{N}\mathbf{O}_{MM}=\mathbf{1} \tag{5.8}$$

and three similar equations.

Truncation to the finite set $n=1, 2,\cdots, M$ is equivalent to replacing the exact unit operator by the approximate or "effective" one:

$$\text{“1”}=|\,\boldsymbol{\phi}\rangle_M\mathbf{N}\langle\boldsymbol{\phi}^\dagger\,|_M, \tag{5.9}$$

i.e., ignoring $\mathbf{X}$ everwhere. This gives

$$\mathcal{G}\approx|\,\boldsymbol{\phi}\rangle_M\mathbf{N}\mathbf{G}\mathbf{N}\langle\boldsymbol{\phi}^\dagger\,|_M, \tag{5.10}$$

$$(\mathbf{N}\mathbf{G}\mathbf{N})\mathbf{A}_{MM}\approx\mathbf{1}, \tag{5.11}$$

so

$$\mathcal{G}\approx|\,\boldsymbol{\phi}\rangle_M\mathbf{A}_{MM}^{-1}\langle\boldsymbol{\phi}^\dagger\,|_M. \tag{5.12}$$

When this approximate form of $\mathcal{G}$ is inserted in the collision matrix, the resulting form is identical to that following from the solution (4.4) of the dynamical equation in Sec. IV.

VI. ARGUMENTS FOR THE SUPERIORITY OF (3.15) IN THE SPECIAL CASE OF TOBOCMAN'S STATES

Tobocman and co-workers have set up a number of different formulas for the collision matrix from a given set of states. Tobocman and Nagarajan[1] (called TN) give two results, viz., (20) and (21); Nagarajan, Shah, and Tobocman[2] (NST) give three formulas corresponding to their Green's functions G_A, G_B, and G_I, and Purcell[3] gives one formula. G_A of NST and (20) of TN are the same. G_B of NST corresponds to the result of the present work, specialized to the particular states ϕ_n used by Tobocman and co-workers, viz., a complete orthogonal set in a region larger than and enclosing the integration region. In the particular case when ϕ_n have this character, it is possible to give further arguments in favor of the result (3.15).

Let us consider the one-body case for definiteness and denote matrix elements over the inner, outer, and total regions by $\langle\ \rangle_0^a$, $\langle\ \rangle_a^R$, $\langle\ \rangle_0^R$, respectively ($R>a$). We can regard the various formulas as corresponding to various extensions of the expanded function ψ into the outer region. Let us call the extension, defined in the outer region (a, R) only, $\mathcal{E}(r)$. Since $|\,\phi_n\rangle$ are orthogonal in $(0, R)$, the coefficients in

$$\psi=\sum_{n=1}^{\infty}d_n\phi_n \tag{6.1}$$

are

$$d_n=\langle\phi_n^\dagger\,|\,\psi\rangle_0^a+\langle\phi_n^\dagger\,|\,\mathcal{E}\rangle_a^R. \tag{6.2}$$

On inserting the expansion of ψ in the right-hand side of (6.2), we get

$$\mathbf{d}=\mathbf{O}\mathbf{d}+\mathbf{e}, \tag{6.3}$$

where $\mathbf{e}$ is the vector with elements

$$e_n=\langle\phi_n^\dagger\,|\,\mathcal{E}\rangle_a^R.$$

It follows that

$$(\mathbf{1}-\mathbf{O})\mathbf{d}=\mathbf{e} \tag{6.4}$$

and

$$\mathbf{O}\mathbf{e}=0. \tag{6.5}$$

The second equation is expected since

$$(\mathbf{O}\mathbf{e})_m=\sum_n\langle\phi_m^\dagger\,|\,\phi_n\rangle_0^a\langle\phi_n^\dagger\,|\,\mathcal{E}\rangle_a^R$$

$$=0,$$

since

$$\sum_n\phi_n(r)\phi_n(r')=\delta(r-r').$$

The first equation cannot be solved for $\mathbf{d}$ since $(\mathbf{1}-\mathbf{O})$ for Tobocman states has no inverse. This is also expected, since no dynamics have been introduced. The relation $(\mathbf{1}-\mathbf{O})\mathbf{d}=\mathbf{e}$ is merely a condition on the

solution **d** obtained from the dynamical equations

$$(H+\mathfrak{L}-E)\,|\psi\rangle=\mathfrak{L}\,|\psi\rangle$$

or

$$\langle\psi^\dagger\,|\,H+\mathfrak{L}-E\,|\,\phi_n\rangle_0{}^a=\langle\phi_n{}^\dagger\,|\,\mathfrak{L}\,\psi\rangle_0{}^a,$$

whence,

$$(E_n-E)\langle\phi_n{}^\dagger\,|\,\psi\rangle_0{}^a+\langle\psi^\dagger\,|\,H'+\mathfrak{L}\,|\,\phi_n\rangle_0{}^a = \langle\phi_n{}^\dagger\,|\,\mathfrak{L}\,|\,\psi\rangle_0{}^a,$$

where $(H-H')$ is the Hamiltonian of the ϕ_n, so

$$\sum_m\left[(E_n-E)\delta_{nm}+\langle\phi_m{}^\dagger\,|\,H'+\mathfrak{L}\,|\,\phi_n\rangle_0{}^a\right]d_m = \tfrac{1}{2}g_n+(E_n-E)e_n. \quad (6.6)$$

Depending on the choice for $\mathcal{E}(r)$, i.e., for e_n, these equations can be solved for d_n. On using $\mathbf{d}=\mathbf{Od}+\mathbf{e}$, it can easily be seen that this set of equations is equal to the set obtained by direct substitution of

$$\Psi=\sum_n d_n\phi_n$$

in the second equation, viz.,

$$\mathbf{A}_\infty\mathbf{d}=\tfrac{1}{2}\mathbf{g}, \quad (6.7)$$

where $\mathbf{A}_\infty$ is the complete matrix of $A\equiv(H+\mathfrak{L}-E)$. Since this equation contains no reference to $\mathcal{E}$ or e, whereas we know that the solution **d** depends on $\mathcal{E}$, we conclude that $\mathbf{A}_\infty$ has no inverse, so that this last equation has many solutions **d**. [In the case when the ϕ_n are eigenstates of H, this is obvious, since $\mathbf{A}_\infty{}^{-1}\mathbf{g}$ contains the inverse of $(\mathbf{H}-\mathbf{E})=\mathbf{O}(\mathcal{E}-\mathbf{E})$ and $\mathbf{O}^{-1}$ does not exist.]

While all solutions **d** corresponding to all forms $\mathcal{E}(r)$ must lead to the same results for U when all states are retained, this is no longer true when sums are truncated. In this case, different choice of $\mathcal{E}$ give different results, and it is important to choose the best form.

Properties of Truncated Forms

The choice of $\mathcal{E}(r)$ implicitly made in TN (20) and in G_A of NST is $\mathcal{E}(r)=0$, i.e., $\mathbf{e}=0$. The choice of $\mathcal{E}(r)$ corresponding to the stationary form (3.15) of the present paper (which coincides with G_B of NST) is that $\mathcal{E}(r)$ should be the extrapolation of the finite-series approximation for Ψ (viz., $\Psi=\sum^m{}_{n=1}d_n\phi_n$) into the outer region. This means

$$e_n=\sum_m d_m\langle\phi_n{}^\dagger\,|\,\phi_m\rangle_a{}^R = d_n-\sum_m d_m O_{nm}. \quad (6.8)$$

It directly follows that the above equation for **d** reduces to the variation-principle form

$$\mathbf{A}_{MM}\mathbf{d}=\tfrac{1}{2}\mathbf{g}. \quad (6.9)$$

From this analysis we may conclude that the latter choice gives better results than the former, since the choice $\mathcal{E}(r)=0$ implies a discontinuity at $r=a$ in Ψ, and any finite series for Ψ will be distorted by this discontinuity. (The value of Ψ will be particularly poor near $r=a$ because it will tend to have the mean of the two values at the discontinuity). In contrast, the latter choice of $\mathcal{E}(r)$ makes $\Psi(r)$ smooth across $r=a$. *In fact, it is the smoothest possible systematic choice. In this sense, we suggest that there is no systematic recipe for U that is better than the stationary form* (3.15).

Statement of Relative Merits in Terms of Green's Functions

Purcell[3] has noted an aternative view of the choice $\mathcal{E}(r)=0$. This stems from the observation that the expansion of the wave function may often be stated in terms of Green's functions. Since Green's functions are such that they have a discontinuity in derivative at the point when the two arguments are equal, it follows that theories involving such equal-argument derivatives will be inferior to those that do not.

We define $G^{(R)}(r,r')$ as the Green's function corresponding to the operator $G^{(R)}\equiv[H+\mathfrak{L}^{(R)}(b)-E]^{-1}$, where superscript (R) on $\mathfrak{L}$ denotes that $\mathfrak{L}$ contains $\delta(r-R)$, and superscript (R) on $G^{(R)}(r,r')$ denotes that it applies to all $r,r'\leq R$. We have

$$[H_r+\mathfrak{L}^{(R)}(b)-E]G^{(R)}(r,r')=r^{-2}\delta(r-r') \quad (6.10)$$

or

$$G^{(R)}(r,r')=\sum_\lambda^\infty\frac{\langle r\,|\,\phi_\lambda\rangle\langle\phi_\lambda{}^\dagger\,|\,r'\rangle}{E_\lambda-E}, \quad (6.11)$$

where the states $|\,\phi_\lambda\rangle$ are eigenstates of $H+\mathfrak{L}^{(R)}(b)$. The discontinuity in the derivative stems from the source δ function, and has magnitude

$$\frac{dG^{(R)}}{dr}(r,r')\Bigg|_{r=r-\prime}^{r=r+\prime}=-\left(\frac{2m}{\hbar^2r^2}\right); \quad (6.12)$$

we now discuss four theories in the light of this criterion.

Example 1: An example of a recipe which is poor in terms of the present criterion is that of TN (20) or, equivalently, G_A of NST. This G_A is, in fact, equal to $G^{(R)}$. When $\mathcal{E}=0$, the extended wave function ψ may be written [see (20) of TN]

$$\left(\frac{2M}{\hbar^2a^2}\right)\psi(r')=\psi(a)\left[\frac{dG^{(R)}}{dr}(r,r')\right]_{r=a} -[(\psi)']_{r=a}G^{(R)}(a,r'). \quad (6.13)$$

One sees that the discontinuity in the derivative of G is directly responsible for the discontinuity in $\psi(r')$ at $r'=a$. The collision matrix is obtained by evaluating

$\psi(a)$ on putting $r'=a$, so we see that the "dangerous" quantity $[(dG/dr)(r,a)]_{r=a}$ occurs.

Equation (21) of TN is even worse, since it involves differentiating this formula for $\psi(r')$ at $r'=a$. While (20) is poor for a truncated series, it is exact for an untruncated case provided dG/dr is evaluated from inside $r=a$. In contrast (21) fails even for the untruncated case.

Example 2: R-matrix theory, where there is no outside region, i.e., $R=a$. In this case, the standard result of R-matrix theory may be stated:

$$\psi(r)=(\hbar^2a/2m)G^{(a)}(r,a)[(r\psi)'_{r=a}-b\psi(a)], \quad (6.14)$$

where

$$G^{(a)}(r,r')=\langle r\mid[H+\mathfrak{L}^{(a)}(b)-E]^{-1}\mid r'\rangle$$
$$=\sum_\lambda^\infty \frac{\langle r\mid\phi_\lambda\rangle\langle\phi_\lambda{}^\dagger\mid r'\rangle}{E_\lambda-E}.$$

As we know, one makes an error if one tries to obtain $\psi'(a)$ by differentiating this formula at $r=a$. This erroneous procedure gives $(r\psi)'_{r=a}=b\psi(a)$, while the correct answer is

$$\psi'(a)=\psi(a)\{-(\hbar^2a/2m)G^{(a)}(a,a)]^{-1}+b\}.$$

This discrepancy exactly corresponds to the discontinuity in dG/dr. We have

$$\left[\frac{d}{dr}[rG^{(a)}(r,a)]\right]_{r=a}=bG^{(a)}(a,a)=\frac{b\psi(a)(2m/\hbar^2a)}{(r\psi)'_{r=a}-b\psi(a)},$$

$$\left[\frac{d}{dr}[rG^{(a)}(r,a)]\right]_{r=a-}=\frac{(r\psi)'_{r=a}(2m/\hbar^2a)}{(r\psi)'_{r=a}-b\psi(a)}.$$

The difference is the expected value $-2m/\hbar^2a$. While it is wrong to differentiate this form of $\psi(r)$ at $r=a$, it is correct to evaluate $\psi(r)$ at $r=a$ since no derivative of G appears.

Example 3: Purcell proposes a method for avoiding the "dangerous" quantity

$$[(dG^{(R)}/dr)(r,a)]_{r=a}.$$

He retains the choice $\mathcal{E}(r)=0$, which implies the above equation:

$$\frac{2m}{\hbar^2a^2}\psi(r')=\psi(a)\left[\frac{dG^{(R)}(r,r')}{dr}\right]_{r=a}-(\psi)'_{r=a}G^{(R)}(a,r'), \quad (6.15)$$

but he evaluates this at a point ($r=a_0$, say) inside $r=a$. (It is assumed that $\mathbf{a}$ is chosen well outside the interaction region, so that a_0 is not inside this region). On inserting $a_0\psi(a_0)=I(a_0)-UO(a_0)$, $a\psi(a)=I(a)-UO(a)$, $(r\psi)'_{r=a}=I'(a)-UO'(a)$, one finds the resulting formula for U (with $a_0<a<R$):

$$U=\frac{I(a)[dG^{(R)}(r,a_0)/dr]_{r=a}-[I'(a)-I(a)]G^{(R)}(a,a_0)-(2m/\hbar^2aa_0)I(a_0)}{O(a)[dG^{(R)}(r,a_0)/dr]_{r=a}-[O'(a)-O(a)]G^{(R)}(a,a_0)-(2m/\hbar^2aa_0)O(a_0)}.$$

An evident weakness of this procedure is that a_0 must be significantly different from a or else the above objection applies. If a_0 is much less than a, it means that the wave-function expansion includes a large region of free space where the wave function ψ has the explicit form $r^{-1}(I-UO)$. It is unlikely that any real improvement can be obtained by extending the expansion region in this way. Furthermore, the objection to the choice $\mathcal{E}=0$ still applies, since there is a discontinuity in ψ at $r=a$, and the expansion of ψ over the entire range is distorted by this discontinuity.

Example 4: the variation-principle recipe, which is equivalent to G_B of NST. It is clearly important to check whether this recipe involves a "dangerous" quantity, either implicitly or explicitly. At first sight, there is trouble. From formulas in Appendix A, we may write the wave function thus:

$$\psi(r)=\tfrac{1}{2}[1+B^{\delta\gamma}(1)-(aO'/O)B^{\gamma\gamma}(1)]^{-1}$$
$$\times\sum_n\langle r\mid\phi_n\rangle[(\mathbf{H}-\mathbf{E})^{-1}\mathbf{g}]_n. \quad (6.16)$$

NST define a so-called Green's function

$$G_B(r,r')=\sum_{n,m}\langle r\mid\phi_n\rangle[(\mathbf{H}-\mathbf{E})^{-1}]_{nm}\langle\phi_m{}^\dagger\mid r'\rangle,$$

so that

$$B^{\gamma\gamma}=(\hbar^2a/2m)G_B(a,a),$$
$$B^{\delta\gamma}=(\hbar^2a/2m)[(d/dr)rG_B(r,a)]_{r=a},$$

and

$$\psi(r)=\left(\frac{\hbar^2a}{2m}\right)\left(I'-\frac{O'}{O}I\right)_{r=a}$$
$$\times\left[1+\frac{\hbar^2a}{2m}\left\{\frac{drG_B(r,a)}{dr}\right\}_{r=a}-\frac{aO'}{O}\frac{\hbar^2a}{2m}G_B(a,a)\right]^{-1}$$
$$\times G_B(r,a), \quad (6.17)$$

we see that, apart from a multiplying factor, $\psi(r)$ involves $G_B(r,a)$ but not its derivative. This checks the fact that $\psi(r)$ has no discontinuity at $r=a$ in the case $\mathcal{E}(r)=\psi(r)$. However, the multiplying factor does involve $[dG_B(r,a)/dr]_{r=a}$, so the theory is apparently subject to the Purcell criticism. However, this conclusion is incorrect, since the function G_B defined above ceases to exist when the sums on n, m include all states. [As previously noted, if $\mid\phi_n\rangle$ are eigenstates of H, then $(\mathbf{H}-\mathbf{E})\propto\mathbf{O}$, and $\mathbf{O}^{-1}$ does not exist when all states are present]. NST do not comment on the fact when they introduce G_B. Thus the function G_B as

defined above does not go over into a proper Green's function when all states n, m are included. For this reason, it follows that the Purcell criticism does not apply. This view is supported by the fact that the above formula for $\psi(r)$ is correct when it specialized to the case $R=a$ (i.e., no outer region):

$$B^{\delta\gamma}(1)=bB^{\gamma\gamma}(1)=bR(b),$$

$$\psi(r)=\left(\frac{\hbar^2 a}{2m}\right)^{1/2}\left(I'-\frac{O'}{O}I\right)_{r=a}\left[1+\left(b-\frac{aO'}{O}\right)R(b)\right]^{-1}\times\sum_\lambda\frac{\langle r\mid\phi_\lambda\rangle\gamma_\lambda}{E_\lambda-E}.$$

This is the standard R-matrix-theory result. Note that G_A of NST *does* become a proper Green's function when all states are included, so that the criticism of this recipe stands.

Conclusions

The essential result is simply that there exists a best formula for the collision matrix in terms of linear combinations of given functions, viz., (3.15) with (3.16). This result follows from the stationary principle of Sec. II, despite the fact that the stationary property fails for linear combinations.

In a practical calculation of a cross section with resonances, the result of this paper can be combined with an independent calculation of the direct interaction (i.e., background) scattering (e.g., from a coupled channel or other direct interaction theory). Once the wave function for such background has been obtained, it may be regarded as one of the states ϕ_n, while the other $(M-1)$ states give rise to local resonances. On forming the matrix $\mathbf{A}$ with all M states included, and then calculating the collision matrix with (3.15) and (3.16) interference effects between the background and resonances are automatically included. An important feature of this approach is that it is unnecessary to orthogonalize states ϕ_n, in particular there is no need for the background state to be orthogonal to the resonance states.

APPENDIX A: ALGEBRAIC MANIPULATIONS GIVING ALTERNATIVE FORMS OF R IN (3.11) AND (3.15)

One-Body Case

There are two varieties of alternative forms:

(*1*) *Variation of boundary condition.* R may be replaced by the corresponding quantity for boundary condition b, viz.,

$$R(b)=\boldsymbol{\gamma}^T[\mathbf{H}+\mathfrak{L}(b)-\mathbf{E}]^{-1}\boldsymbol{\gamma}.$$

Matrix algebra shows the relation to be

$$R=[1-Rb(aO'/O-b)]^{-1}R(b).$$

A related result is that the relative values of the coefficients in $\psi_{t0}=\sum d_n\phi_n$ are unchanged if $\mathfrak{L}$ is replaced by any $\mathfrak{L}(b)$:

$$\mathbf{d}=\tfrac{1}{2}\mathbf{A}^{-1}\mathbf{g}=\tfrac{1}{2}[1-R(b)(aO'/O-b)]^{-1}\times[\mathbf{H}+\mathfrak{L}(b)-\mathbf{E}]^{-1}\mathbf{g}.$$

(*2*) *Removal of* $\mathfrak{L}$ *and varied symmetrization of* $\mathbf{H}$.
Defining $C_{mn}=\langle\phi_m{}^\dagger\mid H-E\mid\phi_n\rangle$, we have

$$C_{nm}-C_{mn}=\gamma_m\delta_n-\gamma_n\delta_m,$$

where

$$\delta_n=(\hbar^2a/2m)^{1/2}(r\phi_n)'_{r=a}.$$

The matrix $\mathbf{D}$ defined by $D_{mn}\equiv[H+\mathfrak{L}(0)-E]_{mn}$ is

$$\mathbf{D}=\alpha(\mathbf{C}+\boldsymbol{\gamma}\boldsymbol{\delta}^T)+(1-\alpha)(\mathbf{C}^T+\boldsymbol{\delta}\boldsymbol{\gamma}^T),$$

and has the properties that it is the same for all α and it is symmetric if $\alpha=\frac{1}{2}$ or if $H+\mathfrak{L}(0)$ is Hermitian. Splitting $\mathbf{D}$ into two parts,

$$\mathbf{D}=\mathbf{Z}+\mathbf{Y},$$

with

$$\mathbf{Z}=\alpha\mathbf{C}+(1-\alpha)\mathbf{C}^T,$$

$$\mathbf{Y}=\alpha\boldsymbol{\gamma}\boldsymbol{\delta}^T+(1-\alpha)\boldsymbol{\delta}\boldsymbol{\gamma}^T,$$

we have

$$\mathbf{Z}^{-1}=(\mathbf{1}+\mathbf{Z}^{-1}\mathbf{Y})\mathbf{D}^{-1}.$$

On defining

$$B^{xy}(\alpha)=\mathbf{x}^T[\alpha(\mathbf{H}-\mathbf{E})+(1-\alpha)(\mathbf{H}^T-\mathbf{E}^T)]^{-1}\mathbf{Y},$$

$$R^{xy}(0)=\mathbf{x}^T[H+\mathfrak{L}(0)-E]^{-1}\mathbf{Y}=\mathbf{x}^TD^{-1}\mathbf{Y}$$

$$[\text{N.B.: } R^{xy}(0)=R^{yx}(0)],$$

we get four equations on putting vectors $\mathbf{x}$, $\mathbf{y}=\boldsymbol{\gamma}$, $\boldsymbol{\delta}$ around the equation for $\mathbf{Z}^{-1}$, the first being

$$B^{\gamma\gamma}(\alpha)=R^{\gamma\gamma}(0)+\alpha B^{\gamma\gamma}(\alpha)R^{\delta\gamma}(0)+(1-\alpha)B^{\gamma\delta}(\alpha)R^{\gamma\gamma}(0).$$

Eliminating $R^{\delta\gamma}(0)$ from this equation and the one for $B^{\delta\gamma}$ gives $R(0)$ in terms of the B's:

$$R^{\gamma\gamma}(0)\equiv R(0)=B^{\gamma\gamma}(\alpha)\{[1+\alpha B^{\delta\gamma}(\alpha)]\times[1+(1-\alpha)B^{\gamma\delta}(\alpha)]-\alpha(1-\alpha)B^{\gamma\gamma}(\alpha)B^{\delta\delta}(\alpha)\}^{-1}$$

$$=B^{\gamma\gamma}(1)/[1+B^{\delta\gamma}(1)].$$

The solutions for B's in terms of R's(0) are

$$B^{\gamma\gamma}(\alpha)=(1-R^{\gamma\delta})^{-1}R^{\gamma\gamma},$$

$$B^{\delta\delta}(\alpha)=(1-R^{\gamma\delta})^{-1}R^{\delta\delta},$$

$$B^{\gamma\delta}(\alpha)=(1-R^{\gamma\delta})^{-1}[R^{\gamma\delta}-\alpha((R^{\gamma\delta})^2-R^{\gamma\gamma}R^{\delta\delta})],$$

$$B^{\delta\gamma}(\alpha)=(1-R^{\gamma\delta})^{-1}[R^{\gamma\delta}-(1-\alpha)((R^{\gamma\delta})^2-R^{\gamma\gamma}R^{\delta\delta})].$$

Note that $B^{\gamma\gamma}$, $B^{\delta\delta}$, $(B^{\gamma\delta}+B^{\delta\gamma})\equiv U$, $(B^{\gamma\delta}-B^{\delta\gamma})\times(1-2\alpha)^{-1}\equiv V$ are independent of α. Further, eliminating all R's, a relation between the B's is found to be

$$V^2-U^2+4V+4B^{\gamma\gamma}B^{\delta\delta}=0.$$

In Sec. III of the text, we mention the value of the logarithmic derivative, f_{t0}(say), obtained by direct differentiation of the sum ψ_{t0}. This is, on using the above kind of manipulations,

$$f_{t0}=[(r\psi_{t0})'/r\psi_{t0}]_{r=a}=B^{\delta\gamma}(1)/aB^{\gamma\gamma}(1).$$

This is to be compared with the form implied by the result (3.11), viz.,

$$f=[aR(0)]^{-1}=[aB^{\gamma\gamma}(1)]^{-1}+B^{\delta\gamma}(1)/aB^{\gamma\gamma}(1),$$

which is clearly different in general.

Another result easily obtainable from the same sort of analysis is that the solution $\mathbf{d}$ may be reexpressed

$$\mathbf{d}=\tfrac{1}{2}\mathbf{A}^{-1}\mathbf{g}=\tfrac{1}{2}\{[\mathbf{1}-(aO'/O)R(0)][\mathbf{1}+B^{\delta\gamma}(1)]\}^{-1}\times(\mathbf{H}-\mathbf{E})^{-1}\mathbf{g}.$$

The Many-Body Case

The generalizations of the above algebraic relations for the one-body case are easily shown to be

$$\mathbf{R}=\mathbf{R}(b)[\mathbf{1}-(\mathbf{a}\mathbf{O}'/\mathbf{O}-\mathbf{b})\mathbf{R}(b)]^{-1},$$

where $\mathbf{a}(\mathbf{O}'/\mathbf{O})-\mathbf{b}$ is the diagonal matrix with elements $a_c(O_c'/O_c)-b_c$ and

$$\begin{aligned}\mathbf{R}(0)&=\{\mathbf{1}+(1-\alpha)\mathbf{B}^{\gamma\delta}(\alpha)-\alpha(1-\alpha)\mathbf{B}^{\gamma\gamma}(\alpha)\\&\quad\times[\mathbf{1}+\alpha\mathbf{B}^{\delta\gamma}(\alpha)]^{-1}\mathbf{B}^{\delta\delta}(\alpha)\}^{-1}\mathbf{B}^{\gamma\gamma}(\alpha)[\mathbf{1}+\alpha\mathbf{B}^{\delta\gamma}(\alpha)]^{-1},\\&=\mathbf{B}^{\gamma\gamma}(1)[\mathbf{1}+\mathbf{B}^{\delta\gamma}(1)]^{-1}.\end{aligned}$$

Here we have assumed $\mathbf{A}$ to be symmetric so that the definition (3.16) of $\mathbf{R}$ becomes $\boldsymbol{\gamma}^T\mathbf{A}^{-1}\boldsymbol{\gamma}$. When $\mathbf{A}$ is not symmetric, and (3.16) applies, then the equation for $\mathbf{R}(0)$ is valid only for evaluation of $\alpha=\frac{1}{2}$. In this case, the quantities $B^{\gamma\gamma}$, $B^{\delta\delta}$, U, and V are no longer independent of α.

APPENDIX B: PROPERTIES OF THE OVERLAP MATRIX O FOR A COMPLETE SET

If the $|\phi_n\rangle$ are complete, one form of the unit operator is the diagonal one:

$$1=\sum_n|\phi_n\rangle P_n\langle\phi_n{}^\dagger|.$$

It follows that

$$\mathbf{O}=\mathbf{OPO},$$

where $\mathbf{O}$ is the overlap matrix

$$O_{mn}=\langle\phi_m{}^\dagger|\phi_n\rangle$$

and $\mathbf{P}$ is the diagonal matrix of the P's. By renormalizing the $|\phi_n\rangle$ or by working with $\mathbf{O}'\equiv\mathbf{P}^{1/2}\mathbf{O}\mathbf{P}^{1/2}$, we may suppress P (the same is true in the text if we work with $\mathbf{N}'\equiv\mathbf{P}^{1/2}\mathbf{N}\mathbf{P}^{1/2}$, etc.). Thus consider

$$\mathbf{O}^2=\mathbf{O}.$$

On writing this in terms of the submatrices,

$$\begin{aligned}\mathbf{O}_{Mr}\mathbf{O}_{rM}&=\mathbf{O}_{MM}-\mathbf{O}_{MM}{}^2,\\\mathbf{O}_{MM}\mathbf{O}_{Mr}+\mathbf{O}_{Mr}\mathbf{O}_{rr}&=\mathbf{O}_{Mr},\\\mathbf{O}_{rM}\mathbf{O}_{MM}+\mathbf{O}_{rr}\mathbf{O}_{rM}&=\mathbf{O}_{rM},\\\mathbf{O}_{rM}\mathbf{O}_{Mr}&=\mathbf{O}_{rr}-\mathbf{O}_{rr}{}^2.\end{aligned}$$

If we define

$$\mathbf{W}=\mathbf{O}_{rr}-\mathbf{O}_{rM}\mathbf{O}_{MM}{}^{-1}\mathbf{O}_{Mr},$$

these relations show that

$$\mathbf{W}^2=\mathbf{W},\qquad\mathbf{O}_{rr}\mathbf{W}\mathbf{O}_{rr}=\mathbf{W},$$

$$\mathbf{O}_{Mr}\mathbf{W}=\mathbf{W}\mathbf{O}_{rM}=0.$$

On comparing with the relation satisfied by $\mathbf{X}$ in the text,

$$\mathbf{O}_{rr}\mathbf{X}\mathbf{O}_{rr}=\mathbf{O}_{rr}-\mathbf{O}_{rM}\mathbf{O}_{MM}{}^{-1}\mathbf{O}_{Mr}=\mathbf{W},$$

we see that a solution for $\mathbf{X}$ is

$$\mathbf{X}=\mathbf{W},$$

and that this satisfies the conditions $\mathbf{O}_{Mr}\mathbf{X}=\mathbf{X}\mathbf{O}_{rM}=0$. Further, if $\mathbf{O}_{rr}{}^{-1}$ exists, this solution is unique. In general, $\mathbf{O}$ and $\mathbf{X}$ are projectors, while $\mathbf{O}_{MM}$, $\mathbf{O}_{rr}$ are not.