Stationary bounds on eigenphase shifts: Target wave functions imprecisely known

Robert Blau,*† Leonard Rosenberg,‡ and Larry Spruch*
Department of Physics, New York University, New York, New York 10003
(Received 9 June 1975)

Stationary bounds are obtained on the K matrix, which is characterized by eigenphase shifts and mixing parameters that describe the scattering process. It is assumed that the incident particle is distinguishable from the target particles, and that if there are any open channels apart from the ground state, they are excitation channels. The new development is the omission of the requirement that the wave functions and energies of the target states associated with open channels be known exactly. A stationary lower bound is obtained by using the close-coupling approximation and forming a stationary bound on the matrix potential which arises in that approximation. Stationary upper *and* lower bounds are obtained by the development of stationary upper and lower bounds on the full (exact) optical-model potential; the effects of virtual rearrangements can be included in the latter approach. The stationary bounds derived are rigorous if the calculation is sufficiently accurate so that the bounds on the tangent of each eigenphase lie on the correct branch. This requirement exists in much the same way as in earlier work, which provided calculable bounds only when the target wave functions are known precisely. It is not a new feature of the present paper, whose principal concern is the extension of this earlier work to cases where such precise information about the target is lacking.

I. INTRODUCTION

In recent work, techniques for obtaining stationary upper bounds on scattering lengths, which are applicable when the target wave functions and energies are known precisely,[1] were extended to cases where such precise information about the target is lacking.[2,3] The methods are in essence very simple. At zero incident energy, standard variational principles either directly provide a stationary upper bound on the scattering length, or can readily be modified to do so. If the target wave functions and energies are imprecisely known, the stationary upper bound is only a formal one, since it contains matrix elements which involve the exact target wave functions and exact target energies. However, it was shown[2,3] that all of the imprecisely known matrix elements that occur can be replaced by appropriate stationary bounds, thus yielding the desired calculable stationary upper bound on the scattering length.

The method, unfortunately, cannot be used to obtain stationary bounds on the phase shifts that characterize scattering at nonzero incident energies, since the second-order error term which represents the difference between the true and the variational estimates, and which is given only formally, contains an operator which has a continuum of negative energy as well as positive energy eigenvalues, and is much more difficult to bound.

In seeking stationary bounds on scattering parameters at nonzero incident energies for systems having imprecisely known target states, a natural first step is to examine the close-coupling approximation equations; when precise information about the target is available, these equations, under specified conditions, provide a lower stationary bound on the K-matrix.[4] The question arises as to whether the techniques for bounding matrix elements involving the true target wave functions cannot be used here also, when precise target information is lacking. Indeed, it will shortly be seen that this can be done quite readily for situations in which only excitation channels are open and in which exchange or rearrangement channels need not be considered. In such cases, the "matrix potential" $\underline{V}$ of the close coupling equations has elements which, although imprecisely known, may readily be bounded.

One begins by obtaining stationary bounds on the individual elements of $\underline{V}$ by techniques previously described,[2,5] and continues by constructing an explicit matrix $\underline{U}$ for which $\underline{U} \geq \underline{V}$. The monotonicity theorem may be invoked to provide a bound on the eigenphase shifts; the bound will be a stationary one if U has been so constructed that the elements of $U - \overline{V}$ are second order quantities.

The construction of the matrix $\underline{U}$ turns out to be a simple matter once the stationary bounds on the elements of $\underline{V}$ have been obtained, and the method of construction is given in Sec. II. The technique is admirably suited to problems in which the first few open channels are all excitation channels, but there are not too many problems for which that is the case; an example would be e^+-Li^+ scattering. (The method is equally adaptable to Coulombic potentials, provided suitable boundary conditions are imposed.) Normally, however, as in e^+-He scattering, the energy for positronium formation lies below the first excited state. The technique is rather more limited for the latter problem. The method is often well suited to the static approxi-

mation in which only the target ground state appears, but in an attempt to include virtual positronium formation $\underline{V}$ becomes nonlocal and the method given for constructing $\underline{U}$ fails.

In order to obtain more satisfactory stationary bounds on systems such as this (i.e., systems having rearrangement channels which, while closed at the energy of interest, nevertheless play an important role through virtual excitation), a different procedure is adopted in Sec. III. Assuming that elastic scattering is the only allowable process, or, if additional channels are open that they represent excitation channels, we write Schrödinger's equation as an effective one-body equation for $P\Psi$, where P projects onto the open channel, and bound the optical-model potential. The procedure is computationally more difficult than that given in Sec. II, but has the advantage, in contradistinction to the procedure of Sec. II, that it can in principle converge on the exact answer. It is therefore capable of giving satisfactory results for problems such as positron-atom scattering below the positronium pickup threshold. Above the positronium threshold, or for electron-atom scattering, this method too breaks down, because the operators which must be bounded become nonlocal.

As in the method of Sec. II, problems such as the scattering of positrons by positive ions can be handled by imposing Coulombic boundary conditions. In the case of negative ions, however, the positronium formation channel will be open at all energies; so this case must be excluded.

As in all previous work on bounds on scattering parameters, certain conditions must be met in order for the bounds to be rigorous. The number of Q-space bound states (i.e., eigenvalues below the continuum threshold of the closed-channel part of the Hamiltonian) must be correctly determined, for one thing. Also, we must be sure that the bounds fall on the correct branch of the eigenphase shift tangents. This is discussed in some detail in Sec. IV. We emphasize, however, that all of these questions are inherent in the nature of the variational bound procedure and have been studied before.[4,6,7] They are not new questions that have arisen in conjunction with the present work; i.e., they are not connected with the lack of precise knowledge about the target, which is the central concern of this paper.

It might also be remarked that, in addition to the aforementioned examples, the methods to be presented should often prove useful in obtaining rigorous bounds on scattering parameters for model systems. Such models are particularly important in many-electron atomic or molecular problems, which are too difficult to be handled as they stand. One might, for example, want to treat the inner shells by the use of pseudostates. The use of rigorous stationary bounds on the model problem can help to disentangle the errors involved in solving the model problem from the errors inherent in the model.

II. BOUNDS ON THE POTENTIAL MATRIX: EXCITATION CHANNELS ONLY

Consider a system consisting of a distinguishable particle incident on a spherically symmetric target, the latter being described by a target Hamiltonian H_T, so that the Schrödinger equation for the problem is

$$[H(\vec{r},\vec{q})-E]\Psi(\vec{r},\vec{q}) = [T(\vec{q})+H_T(\vec{r})+V(\vec{r},\vec{q})-E]\Psi(\vec{r},\vec{q})=0, \tag{2.1}$$

where T is the kinetic-energy operator for the projectile, V describes the interaction between the projectile and the target, and E is the total energy of the system. $\vec{q}$ represents the projectile coordinates, and $\vec{r}$ stands for all the target space and spin coordinates. Suppose the normalized target wave functions are $\psi_{T0}(\vec{r}), \psi_{T1}(\vec{r}), \ldots$, with corresponding energy eigenvalues $E_{T0}, E_{T1}, \ldots$, and suppose that there are N open channels. Then the "close-coupling reaction matrix" $\underline{K}_V^P$ is determined by solving the $M \geq N$ coupled equations that result from doing a partial-wave decomposition and approximating the solution to (2.1) by a sum over M target wave functions (including all N open channels) with coefficients $u_i(\vec{q})$; the superscript P denotes the fact that the approximation limits the wave function to lying in P space, while the subscript V denotes the interaction under consideration. The result may be expressed

$$[T(\vec{q})\underline{1}+\underline{V}(\vec{q})+(E\underline{1}-\underline{E}_T)]\underline{u}(\vec{q})=0. \tag{2.2}$$

In Eq. (2.2) $\underline{u}(\vec{q})$ is a column vector consisting of M functions $u_i(\vec{q})$, $i=0,1,\ldots,M-1$, the symbol $\underline{1}$ represents the unit $M\times M$ matrix, $\underline{E}_T$ is the diagonal matrix with elements E_{Ti}, and $\underline{V}(\vec{q})$ is the $M\times M$ matrix whose ijth element is

$$V_{ij}=V_{ij}(\vec{q})=\int \psi_{Ti}^*(\vec{r})V(\vec{q},\vec{r})\psi_{Tj}(\vec{r})\,d\vec{r}=V_{ji}^*. \tag{2.3}$$

The eigenphase shifts determined from (2.2) represent lower stationary bounds on the exact eigenphase shifts[4]; we write this conditionally as

$$\underline{K}\geq\underline{K}_V^P, \tag{2.4}$$

although it must be borne in mind that the inequality on the tangents of the eigenphase shifts implied by (2.4) is valid only when the calculation is suf-

ficiently accurate that we are assured of being on the correct branch. (See below, Sec. IV.)

If the target wave functions ψ_{Ti} are not known exactly, Eq. (2.2) cannot be written down explicitly. However, if we can construct a calculable Hermitian matrix $\underline{U}=\underline{U}(\vec{q})$ satisfying

$$\underline{U}(\vec{q})-\underline{V}(\vec{q})\geq 0 \tag{2.5}$$

for all $\vec{q}$ then the eigenphase shifts corresponding to the K matrix, $\underline{K}_U^P$, obtained by solving the equations that result when $\underline{V}$ is replaced by $\underline{U}$ in (2.2), will, by the monotonicity theorem, represent bounds on the eigenphase shifts corresponding to $\underline{K}_V^P$ and hence in turn to those corresponding to $\underline{K}$;[8] the bound will be stationary if $\underline{U}-\underline{V}$ is of second order. Thus, under the same proviso noted after Eq. (2.4), we will have

$$\underline{K}\geq\underline{K}_V^P\geq\underline{K}_U^P. \tag{2.6}$$

(This inequality also provides stationary bounds on linear combinations of the mixing parameters.) The remainder of this section will accordingly be devoted to the construction of a calculable matrix $\underline{U}(\vec{q})$ satisfying (2.5).

The first step is to compute stationary upper and lower bounds on all the matrix elements defined by (2.3); methods for constructing such bounds have been given previously.[2,5] The matrix $\underline{U}$ is then to be constructed in terms of the quantities $V_{ij}^{(\pm)}$. (We will write $C^{(+)}$ for an upper bound and $C^{(-)}$ for a lower bound on some number, function, or operator C. For a complex function, the bounds are, separately, on the real and imaginary parts. (See below.)

A necessary and sufficient condition for a Hermitian matrix to be positive definite is that the determinants of all of its principal minors be positive.[9] For $M=1$, for which we must have $N=1$, our result is obtained trivially: $\underline{U}$ consists of the single element $V_{00}^{(+)}$ plus some arbitrary positive function $A_{00}(\vec{q})$ which can be varied to give the best bound. It is clear, however, for the case $M=1$, that the optimum value will be $A_{00}=0$.

Consider the case $M=2$. (We must then have $N=1$ or 2.) There are now two conditions that must be satisfied, viz.,

$$U_{00}-V_{00}\geq 0, \tag{2.7a}$$

$$(U_{00}-V_{00})(U_{11}-V_{11})-|U_{01}-V_{01}|^2\geq 0. \tag{2.7b}$$

If $V_{00}^{(+)}$ is the best available stationary bound on V_{00}, then from (2.7a) it is natural to choose U_{00} to be of the form

$$U_{00}=V_{00}^{(+)}+A_{00}, \tag{2.8}$$

where A_{00} is some non-negative decaying function of $\vec{q}$. We will attempt to find a U_{11} which is of the same form as (2.8), that is, we write

$$U_{11}=V_{11}^{(+)}+B_{11}. \tag{2.9}$$

(All of the quantities A_{ii} and B_{ii} will always be non-negative decaying functions of $\vec{q}$.) Substitution of (2.8) and (2.9) into (2.7b) yields

$$|U_{01}-V_{01}|^2\leq(\delta^+V_{00}+A_{00})(\delta^+V_{11}+B_{11}), \tag{2.10}$$

where we have defined the non-negative functions

$$\delta^+V_{jj}\equiv V_{jj}^{(+)}-V_{jj}. \tag{2.11}$$

These are unknown, but all that we have to do in order to ensure that (2.10) is satisfied is to satisfy the inequality

$$|U_{01}-V_{01}|^2\leq A_{00}B_{11}. \tag{2.12}$$

Defining

$$V_{ij}^{(\pm)}\equiv(\mathrm{Re}\,V_{ij})^{(\pm)}+i(\mathrm{Im}\,V_{ij})^{(\pm)}=(V_{ji}^{(\pm)})^*,$$

we simply choose $U_{01}=V_{01}^{(+)}$, and note that the inequality (2.12) will certainly be satisfied if

$$B_{11}=(|v_{01}|^2/A_{00})+A_{11}, \tag{2.13a}$$

where A_{11} is some other non-negative function, and where

$$v_{ij}\equiv V_{ij}^{(+)}-V_{ij}^{(-)}, \tag{2.13b}$$

for all i and j; v_{ij} is the difference of two stationary bounds and is therefore of second order.

For the case $M=1$, we saw that the best value of A_{00} was zero. By the monotonicity theorem, this will give the largest value of the eigenphase shifts associated with $\underline{K}_U^P$. For $M=2$, it is no longer possible to choose $A_{00}=0$ (unless $v_{01}=0$, implying that the target wave functions are known exactly), since we do not want B_{11} to be infinite. Rather, we can vary A_{00} to maximize $\underline{K}_U^P$. However, since the determinant of $\underline{U}-\underline{V}$ depends linearly on A_{11} (with positive coefficient), it is clear that for $M=2$ the best value of A_{11}[i.e., the value which minimizes $\det(\underline{U}-\underline{V})$] is zero. Thus a matrix which bounds $\underline{V}$ for the 2×2 case is

$$\underline{U}=\begin{pmatrix} V_{00}^{(+)}+A_{00} & V_{01}^{(+)} \\ V_{10}^{(+)} & V_{11}^{(+)}+|v_{01}|^2A_{00}^{-1} \end{pmatrix},\quad A_{00}>0. \tag{2.14a}$$

Note that, while any rapidly decaying positive-definite function A_{00} will be sufficient to ensure (2.5), and thus (2.6), a more stringent requirement must be imposed if the latter is to represent a stationary bound. We saw previously that this will only happen if the elements of $\underline{U}-\underline{V}$ are second-order quantities. Since all the $V_{ij}^{(\pm)}$ are stationary bounds, it is clear that $\underline{U}$ will have the desired stationary properties if A_{00} and $|v_{01}|^2A_{00}^{-1}$ differ from zero by second-order quantities. An ob-

vious possibility for A_{00} is $\alpha|v_{01}|$, where α is a parameter which can be varied, with the restriction that it be positive. With this choice, the matrix $\underline{U}$ which we have constructed in (2.14a) becomes

$$\underline{U}=\begin{pmatrix} V_{00}^{(+)}+\alpha|v_{01}| & V_{01}^{(+)} \\ V_{10}^{(+)} & V_{11}^{(+)}+\alpha^{-1}|v_{01}| \end{pmatrix}. \tag{2.14b}$$

The simplest choice is $\alpha=1$; the calculation should be insensitive to α, for α of the order unity, since only second-order quantities are involved. This can be checked, if desired, by repeating the calculation for a few different values of α. The generalization of Eq. (2.14a) to the case of arbitrary M will be found in Appendix A. The $M\times M$ matrix $\underline{U}$ which is constructed there, and of which (2.14b) is a special case, has $V_{ij}^{(+)}$ as its off-diagonal elements. Its diagonal elements are of the form $V_{ii}^{(+)}$ plus sums of second-order quantities involving the known v_{ij}'s, and which, in general, may be multiplied by positive-definite numbers α_i which may be varied to produce the best stationary bound. The matrix $\underline{U}$ is therefore calculable, and in addition to satisfying (2.5) will be Hermitian (so that unitarity is satisfied), and will be a stationary approximation to $\underline{V}$ [i.e., a matrix element of $\underline{U}$ will differ by at most second order from the corresponding (unknown) matrix element of $\underline{V}$]. It will be clear from the derivation given in Appendix A that there is nothing unique about this matrix to be constructed, but we believe that the scheme presented is among the simplest. In particular, there is considerable arbitrariness in the form of the positive second-order quantities which are added to the $V_{ii}^{(+)}$ to form the diagonal elements, and also in the number of positive parameters α_i which may be chosen as multiplicative factors of these positive second-order quantities.

As mentioned above, it would be possible to extend the foregoing approach to take into account the effect of closed channels more generally by adding correlation terms to the sum over target states in the trial wave function. It is easy to show that the addition of such correlations is equivalent to the replacement of the nonlocal part of the optical-model potential by a separable approximation. Since the formulation is considerably simpler when expressed in terms of bounds on the optical potential, it is this subject that we turn our attention to next.

III. STATIONARY BOUNDS ON THE OPTICAL-MODEL POTENTIAL

We consider a scattering system identical to that of Sec. II, but we drop all restrictions on the form of the trial wave function. This means that, in addition to the virtual excitation allowed in Sec. II, we can now, for example, also include virtual rearrangement processes. (As in Sec. II, we continue to assume that the incident particle is distinguishable and that there are no rearrangement channels open.) For simplicity, we will initially assume that the total energy of the system lies below the inelastic threshold, although it will shortly become apparent that this restriction can be removed if only excitation channels are open. We shall also, as in Sec. II, assume that the target ground state is spherically symmetric, to avoid the complications of multiple channels for a given angular momentum; this is only a matter of convenience.

A. Stationary lower bound on tanη

We take as our starting point, rather than the Schrödinger equation (2.1), the equivalent equation[4,10]

$$P(H+HQG^{Q}QH-E)P\Psi=0. \tag{3.1}$$

Here, P projects onto the target ground state,

$$P=|\psi_{T0}\rangle\langle\psi_{T0}|, \tag{3.2a}$$

while Q is defined by

$$Q=1-P. \tag{3.2b}$$

The Green's function G^{Q} is defined as

$$G^{Q}=1/Q(E-H)Q. \tag{3.3}$$

Equation (3.1) is equivalent to

$$(T+V_{00}+v-E_0')u_0=0, \tag{3.4a}$$

where the asymptotic form of u_0 is given by

$$u_0\sim(2\mu/\hbar^2k)^{1/2}(\sin kr-\tan\eta\cos kr),$$

where

$$vu_0\equiv q\int Y_{L0}^{*}(\hat{q})\psi_{T0}^{*}(\vec{r})V(\vec{r},\vec{q})G^{Q}(\vec{r},\vec{q};\vec{r}',\vec{q}') \times V(\vec{r}',\vec{q}')P\Psi(\vec{r}',\vec{q}')\,d\vec{r}\,d\vec{r}'\,d\vec{q}'\,d\hat{q} \tag{3.4b}$$

is a function of q, and where $\vec{q}=q\hat{q}$. We also have

$$P\Psi(\vec{r},\vec{q})=\psi_{T0}(\vec{r})u_0(q)Y_{L0}(\hat{q})/q, \tag{3.4c}$$

and

$$E_0'=E-E_{T0} \tag{3.4d}$$

is the incident kinetic energy of the projectile. [We take E_0' to be given. Since E_{T0} is not known, the total energy E—which is defined by (3.4d)—will have to be replaced by stationary bounds. A similar remark holds for the E_i' in the natural generalization of Eq. (3.4d) when there are several channels open. The remarks of Ref. 8 concerning ranges apply to all such imprecisely known energies.] The other notation in (3.4a) is the same as that introduced in Sec. II.

As in Sec. II, we have done a partial-wave decomposition to arrive at (3.4a). Under our simplifying assumption of elastic scattering from a target in a spherically symmetric ground state, Eq. (3.4a) is a one-dimensional equation in the scalar q; T must be reinterpreted as the operator

$$T=\frac{\hbar^2}{2\mu}\left(-\frac{\partial^2}{\partial q^2}+\frac{L(L+1)}{q^2}\right),$$

where L is the orbital angular momentum of the projectile. The full scattering function is now understood to be proportional to $u_0(q)/q$, as indicated in (3.4c).

In Eq. (3.4a) both V_{00} and v are unknown. If we wish to use the monotonicity theorem as before, we must replace both of these quantities by calculable stationary bounds. It is a straightforward matter to obtain upper and lower stationary bounds[2,5] on V_{00}, which we denote as usual by $V_{00}^{(+)}$ and $V_{00}^{(-)}$, respectively.[11] If, therefore, we can find upper and lower stationary bounds on v, we will be able to compute upper and lower stationary bounds on $\tan\eta$. We are assuming that the accuracy requirements noted in Sec. II and in Sec. IV have been met. Stationary bounds are clearly much more difficult to obtain for v than for V_{00}, since v contains not only the unknown ψ_{T0} but also the unknown G^Q. (The latter is unknown even when ψ_{T0} is known.) It happens that the *upper* stationary bounds on v is the easier one to obtain; most of the work of this section will be concerned with this bound, and hence with a stationary lower bound on $\tan\eta$. The stationary upper bound on $\tan\eta$ will be discussed in Sec. III C.

We begin by considering the spectrum of QHQ. It has a continuum part which is bounded from below by E_{T1}; in addition, there may be ν discrete bound states lying below E_{T1}. If ν is not zero, we must "subtract out" the effects of these low-lying bound states in a manner which has been described previously.[12] The problem of determining ν exists in the present treatment, which is applicable when the target wave functions are not known precisely, in much the same way as it exists in previous work,[4,7] in which the stationary bounds obtained do require knowledge of the exact target wave functions. In other words, the problem of determining ν is not a new feature of the present work, and is not associated with the lack of precise knowledge about the target. We do now, however, have the additional complication that the projection operator Q is not known precisely. The procedure is not, however, essentially different. We first construct a trial projection operator $Q_t=1-|\psi_{T0t}\rangle\times\langle\psi_{T0t}|$. (We shall always use the subscript t to denote trial entities.) The determination of ν then proceeds by constructing ν' orthonormal functions, $\phi_i^{Q_t}$, $i=1,2,\ldots,\nu'$, which diagonalize Q_tHQ_t, and for which the expectation values of Q_tHQ_t with respect to these functions, $\epsilon_i^{Q_t}$, lies below E_{T1}. Provided one has reason to believe that Q_t is close to Q, i.e., that ψ_{T0t} is close to ψ_{T0}, then if the inclusion of a few additional functions to the set fails to result in an additional expectation value below E_{T1} one would make the assumption $\nu=\nu'$. If the value of ν so determined is different from zero, the resulting stationary bound will differ from the $\nu=0$ stationary bound by terms which involve the $\epsilon_i^{Q_t}$, as well as matrix elements between the known $\phi_i^{Q_t}$ and the unknown target wave functions. Such matrix elements may readily be bounded by techniques previously described. We may therefore, for simplicity, assume $\nu=0$ in what follows, since the case of nonzero ν does not involve any essentially new problems. However, it must be understood that the results which are about to be derived are rigorous only if ν has been correctly determined.

If $\nu=0$, G^Q is a nonpositive operator, and satisfies the inequality

$$G^Q\leq\frac{|[Qf_t(\vec{r},\vec{q})]\rangle\langle[Qf_t(\vec{r}',\vec{q}')]|}{\langle f_t|Q(E-H)Q|f_t\rangle},\tag{3.5}$$

where $f_t(\vec{r},\vec{q})$ is any function which is quadratically integrable over the full $\vec{q}$ and $\vec{r}$ space. [The stationary bound aspect of (3.5) will greatly simplify the choice of any parameters contained in f_t; we will return to this point in Sec. III B]. The replacement of G^Q by the right-hand side of (3.5) and the use of the stationary upper bound on V_{00} yields an approximation to Eq. (3.4) which can be written

$$(T+V_{00}^{(+)}+\lambda|F\rangle\langle F|-E_0')|\tilde{u}_0\rangle=0,\tag{3.6}$$

where $F(q)$, the coordinate representation of $|F\rangle$, is

$$F(q)\equiv q\int Y_{L0}^*(\hat{q})\psi_{T0}^*(\vec{r})V(\vec{r},\vec{q})[Qf_t(\vec{r},\vec{q})]\,d\vec{r}\,d\hat{q}\tag{3.7}$$

and where

$$\lambda\equiv\langle f_t|Q(E-H)Q|f_t\rangle^{-1}\tag{3.8}$$

is a number.

If ψ_{T0} and therefore Q are known exactly, then (3.6) (with any f_t) represents a (numerically) solvable one-body equation. In that case, the quantity $\tan\tilde{\eta}$ obtained from (3.6) will be a lower stationary bound on the true value, that is,

$$\tan\eta\geq\tan\tilde{\eta}.\tag{3.9}$$

We are interested, however, in the case where ψ_{T0} is imprecisely known. $F(q)$ and λ will then also be imprecisely known. Proceeding for the moment as if $F(q)$ and λ were known, we rewrite (3.6) as the

integral equation

$$|\tilde{u}_0\rangle = |u_s\rangle + \lambda G_s |F\rangle\langle F|\tilde{u}_0\rangle . \tag{3.10a}$$

Dropping the bra-ket notation formalism, which is useful only for the operator notation of equations such as (3.5), we revert to functional form and write the formal solution of (3.10a) as

$$\tilde{u}_0 = u_s + \frac{(F, u_s)}{1 - \lambda(F, G_s F)} \lambda G_s F. \tag{3.10b}$$

Here, u_s is the regular solution of the modified static approximation equation

$$(T + V_{00}^{(+)} - E_0')u_s = 0, \tag{3.11}$$

and

$$G_s(q, q') = u_s(q_<) u_{s\,\mathrm{irreg}}(q_>) \tag{3.12}$$

is the Green's function associated with (3.11) and satisfies

$$[T(q) + V_{00}^{(+)}(q) - E_0']G_s(q, q') = -\delta(q - q'); \tag{3.13}$$

$u_{s\,\mathrm{irreg}}$ is an appropriately chosen irregular solution of (3.11). Experience shows that one-body equations of the type (3.11) are readily solved numerically; u_s, G_s, and the associated $\tan\eta_s$ can therefore be taken as known. We then have,[13] from the asymptotic form of Eq. (3.10b),

$$\tan\tilde{\eta} = \tan\eta_s + \frac{\lambda |(F, u_s)|^2}{1 - \lambda(F, G_s F)}. \tag{3.14}$$

The last term on the right-hand side of (3.14) is unknown because of the presence of λ and F; the important point, however, is that it consists of matrix elements for which upper and lower stationary bounds can be obtained by techniques previously described. By a suitable choice of upper and lower stationary bounds on these matrix elements, upper and lower stationary bounds on $\tan\tilde{\eta}$ in (3.14) can be calculated. We are concerned at the moment only with the lower stationary bound, and to this end we turn our attention to the last term on the right-hand side of (3.14), and examine the kinds of unknown terms which appear. Using (3.7), (3.2b), and (3.2a), we find that

$$F = F(q) = q \int Y_{L0}^*(\hat{q})\psi_{T0}^*(\vec{r})[V(\vec{r}, \vec{q}) - V_{00}(\vec{q})] \times f_t(\vec{r}, \vec{q})\, d\vec{r}\, d\hat{q}; \tag{3.15}$$

since Q and T operate in different spaces and therefore commute, λ^{-1} defined by (3.8) becomes

$$\lambda^{-1} = \int f_t^*(E - H) f_t\, d\vec{r}\, d\vec{q} + 2\,\mathrm{Re}\int f_t^*(\vec{r},\vec{q})[T + V(\vec{r},\vec{q}) - E_0']\psi_{T0}(\vec{r})\xi(\vec{q})\, d\vec{r}\, d\vec{q} - \int \xi^*(\vec{q})[T(\vec{q}) + V_{00}(q) - E_0']\xi(\vec{q})\, d\vec{q}, \tag{3.16}$$

where

$$\xi(\vec{q}) = \int \psi_{T0}^*(\vec{r}) f_t(\vec{r},\vec{q})\, d\vec{r}. \tag{3.17}$$

It is clear that we can bound the quantities λ and $|(F, u_s)|$ appearing in (3.14) if we can get upper and lower stationary bounds on the quantities V_{00}, F, ξ, and the middle term on the right-hand side of (3.16). All these quantities except the last are of forms which have been studied previously,[2,5] and upper and lower stationary bounds are readily obtained for all of them. This middle term, however, as well as the remaining unknown real term in (3.14), viz.,

$$(F, G_s F) = \int F^*(q) G_s(q, q') F(q')\, dq\, dq' = \int q' Y_{L0}^*(\hat{q})\psi_{T0}^*(\vec{r})[V(\vec{r},\vec{q}) - V_{00}(q)] \times f_t^*(\vec{r},\vec{q}) G_s(q,q') f_t(\vec{r}',\vec{q}') q'^{-1} Y_{L0}(\hat{q}') \times [V(\vec{r}',\vec{q}') - V_{00}(q')]\psi_{T0}(\vec{r}')\, d\vec{r}\, d\vec{r}'\, d\vec{q}\, d\vec{q}', \tag{3.18}$$

are of a somewhat different form, but both may be handled in the same way. If we integrate over $\vec{q}$ and $\vec{q}'$, both of these terms are of the form

$$\int \psi_{T0}^*(\vec{r}) W(\vec{r},\vec{r}')\psi_{T0}(\vec{r}')\, d\vec{r}\, d\vec{r}', \tag{3.19}$$

where $W(\vec{r},\vec{r}')$ is known. A quantity of this type may be bounded by using previously described techniques for bounding inner products of the form

$$(\chi, \psi_{T0}), \tag{3.20}$$

where χ is any known quadratically integrable function. We first choose

$$\chi = \chi(\vec{r}') = \int \psi_{T0}^*(\vec{r}) W(\vec{r},\vec{r}')\, d\vec{r} \tag{3.21}$$

and treat χ as known. Now (3.19) is of the form (3.20) and formal stationary upper and lower bounds may be obtained. The bounds are formal because they contain matrix elements involving $\psi_{T0}(\vec{r})$. However, these matrix elements will all either be of the form (3.20) or else of the form

$$\int \psi_{T0}^*(\vec{r}) W'(\vec{r}) \psi_{T0}(\vec{r})\, d\vec{r}, \tag{3.22}$$

where W' is known, for which upper and lower stationary bounds can also be found.[2,5] There is, in fact, more than one way of bounding matrix elements of the forms (3.20) and (3.22), and it might be remarked that the techniques described in Ref. 3, which involve only variational estimates of these forms together with bounds on quantities of

the type

$$\mathfrak{D}(B) \equiv (Q\psi_{T0t}, BQ\psi_{T0t}), \tag{3.23}$$

appear to offer advantages in this case over the techniques of Ref. 2. The reason is that stationary bounds on operators of very complicated form can be handled more readily by the techniques of the former than of the latter, since, for example, we may replace B by some simpler operator $B^{(+)}$ without altering the stationary character of the bound.

B. Extremum principle for the choice of f_t

We have not yet discussed the choice of f_t other than to note that it must decay rapidly in both $\vec{q}$ and $\vec{r}$ space. *Any* such form for f_t will preserve the stationary bound; so one might think of choosing some general form for f_t, with open parameters, and varying these parameters to maximize the right-hand side of (3.14) after the unknown quantities have been replaced by the appropriate bounds. Such a procedure, however, is open to two objections.

The first of these is a very practical one. After the necessary bounds on F, ξ, V_{00}, and $\langle F|G_s|F\rangle$ are computed and substituted into (3.14), the result will be a complicated highly nonlinear functional of f_t, as well as of a trial wave function ψ_{T0t}, and a trial auxiliary (Lagrange) function[14-17] L_{T0t} associated with ψ_{T0t}. Because of this form of the bound, all open parameters in f_t, even if introduced linearly, become in effect nonlinear ones; so computationally the maximization process becomes impractical. The same remarks hold for any open parameters in ψ_{T0t} or L_{T0t}, and all three functions should be obtained from auxiliary minimum principles. ψ_{T0t} will be obtained via a Rayleigh-Ritz calculation, and auxiliary minimum principles have been developed[17] for L_{T0t}. We therefore need some similar technique for determining f_t.

First, however, we mention the second difficulty associated with attempting to determine f_t by the maximization procedure mentioned above. This difficulty is of a more subtle nature. The value of f_t which extremizes (3.14) may be thought of as the solution of the highly nonlinear Euler-Lagrange integro-differential equation associated with that equation. It is not quite clear that such an equation will be free of near-singularity difficulties of the type which are encountered in variational principles and which have been studied previously.[17] We would in any event have a rigorous lower bound, but if such near singularities exist, the stationary character of the lower bound will be lost. We therefore turn our attention to computing an f_t by a method which retains the stationary character of the lower bound and which at the same time is demonstrably free of such near singularities.

That it should be possible to utilize an extremum principle for the evaluation of any parameters introduced into f_t is suggested by the fact that f_t arose in an inequality, (3.5), which is a stationary upper bound. Indeed, if Q were known exactly, the extremum principle would be a trivial one. Because Q is *not* known exactly, we will have to take a slightly circuitous route. Thus we compare the operator

$$P(H + HQG^{Q}QH - E)P \tag{3.24}$$

with the operator obtained from (3.24) by substituting the right-hand side of (3.5) for G^{Q}, i.e., with the operator

$$P\left(H + \frac{|H(Qf_t)\rangle\langle(Qf_t)H|}{\langle f_t|Q(E-H)Q|f_t\rangle} - E\right)P. \tag{3.25}$$

There is no choice of f_t which will make the operators (3.24) and (3.25) identical (G^{Q} is not a separable operator). However, we are concerned only with the effect of these operators on Ψ, and we note that the resulting vectors become identical when f_t is chosen to be

$$f = G^{Q}HP\Psi = Q\Psi. \tag{3.26a}$$

This is most readily verified by noting, with the help of (3.26a), that

$$|PHQG^{Q}HP\Psi\rangle = |PHQ\Psi\rangle$$

and also that

$$\frac{|PHQ\Psi\rangle\langle Q\Psi|H|P\Psi\rangle}{\langle\Psi|Q(E-H)Q|\Psi\rangle} = |PHQ\Psi\rangle,$$

since, using (3.26a),

$$\begin{aligned} Q(E-H)Q|\Psi\rangle &= Q(E-H)G^{Q}HP|\Psi\rangle \\ &= QHP|\Psi\rangle \\ &= QV\psi_{T0}u_0Y_{L0}(\hat{q})/q. \end{aligned} \tag{3.26b}$$

Thus the optimum choice of f_t in Eq. (3.5) is the solution of the equation

$$Q(H-E)Qf = -QV\psi_{T0}u_0Y_{L0}(\hat{q})/q. \tag{3.27}$$

Our task has now been reduced to finding a suitable approximation f_t to the function f defined by (3.27). We note that the bound (3.5) is stationary in f_t; it would be desirable to be able to choose for f_t the solution of

$$Q_t(H-E)Q_tf_t = -Q_tV\psi_{T0t}u_{0t}Y_{L0}(\hat{q})/q. \tag{3.28}$$

The bound obtained from (3.14) would then still be a stationary one. Of course, we cannot hope to solve (3.28) exactly. However, it is shown in

Appendix B that if ψ_{T0t} is chosen with sufficient accuracy that

$$E_{T0t} \equiv (\psi_{T0t}, H_T \psi_{T0t}) < E_{T1} - (E - E_{T0})$$

then $Q_t(H_T - E)Q_t$ is positive definite. If, in analogy with our earlier assumption related to the properties of $Q(H-E)Q$, we make the assumption that $Q_t(H-E)Q_t$ has no discrete bound states lying below E (or that these states have been subtracted out), it follows that this operator (or the equivalent operator with a modified Hamiltonian when states have to be subtracted out) is also positive definite. This being the case, it is well known[18] that if the parameters in f_{tt} are chosen by minimization of the functional

$$M(f_{tt}) \equiv (f_{tt}, Q_t(H-E)Q_t f_{tt}) - (f_{tt}, Q_t V \psi_{T0t} u_{0t} Y_{L0}/q) - (Q_t V \psi_{T0t} u_{0t} Y_{L0}/q, f_{tt}), \tag{3.29}$$

f_{tt} will be a variational approximation to f_t. This is the auxiliary minimum principle we have been seeking. We obtain f_{tt} by minimizing the right-hand side of (3.29), and it is this f_{tt} that we use in Eqs. (3.15)–(3.18). The only unknowns appearing in those equations are then the matrix elements containing the target function ψ_{T0}. We bound these matrix elements in accordance with the discussion given in connection with those equations, and these bounds are used in (3.14) to obtain the desired bound on $\tan\tilde{\eta}$.

We note, finally, that if the target functions are known exactly, so that P and Q are known exactly, the above results would be simplified. It is easy to show that, for P and Q known, one may write, in lieu of (3.14),

$$\tan\tilde{\eta} = \tan\eta^P + \frac{|\langle Qf_t | (H-E)P\Psi^P\rangle|^2}{\langle Qf_t | E - H - (H-E)G^P(H-E) | Qf_t\rangle}, \tag{3.30}$$

where η^P is the phase shift associated with the equation

$$P(H-E)P\Psi^P = 0,$$

and where G^P is the Green's function defined by appropriate boundary conditions and by

$$P(H-E)PG^P = -P.$$

It is clear that (3.30) remains unchanged under the replacement of Qf_t by $(Q+P)f_t$ in both the numerator and denominator of the last term on the right-hand side; hence the additional step of projecting out the P-space part of f_t is unnecessary.[19] This is not true in (3.14), because instead of G^P one finds the Green's function G_s which is associated with the modified static equation (3.11) in which V_{00} is replaced by $V_{00}^{(+)}$. Hence this computational simplification of being allowed to drop Q is not available in the present case. We have seen, however, that the explicit appearance of the Q's in (3.14) can be dealt with so as to retain the stationary bound in a rigorous way, but, of course, the calculations are much more difficult when ψ_{T0} is not known.

C. Stationary upper bound on $\tan\eta$

At the beginning of this section, we made use of the crude upper bound on G^Q,

$$G^Q \le 0,$$

to obtain a stationary upper bound on G^Q, and used that to obtain a stationary lower bound on $\tan\eta$. It is possible to make use of the crude lower bound

$$G^Q \ge 1/(E - E_{T1}) \tag{3.31}$$

to obtain a stationary upper bound on $\tan\eta$. The method of using (3.31) to obtain this bound is not new[20]; the new feature here is that this stationary upper bound on $\tan\eta$, which involves matrix elements involving ψ_{T0}, and hence in general is only a formal bound, may be converted into a calculable bound via the bounds on these imprecisely known quantities, in a manner similar to that described at the beginning of this section.

The starting point is the identity for G^Q (see, e.g., Carew and Rosenberg, Ref. 20), which we now write in the form

$$G^Q = G_t^Q + G_t^{Q\dagger} + G_t^{Q\dagger}Q(H-E)QG_t^Q + \delta G^{Q\dagger}Q(H-E)QG^QQ(H-E)Q\,\delta G^Q, \tag{3.32}$$

where $\delta G^Q \equiv G_t^Q - G^Q$, and where we have inserted a factor of unity in the form of $-Q(H-E)QG^Q$ in the last term on the right-hand side. Using (3.31) in the second-order term m(3.32), one obtains

$$G^Q \ge G_v^Q,$$

where

$$G_v^Q = G_t^{Q\dagger} + G_t^Q + G_t^{Q\dagger}Q(H-E)QG_t^Q - (E_{T1}-E)^{-1}[G_t^{Q\dagger}Q(H-E)Q + Q(H-E)QG_t^Q + G_t^{Q\dagger}Q(H-E)Q(H-E)QG_t^Q + Q]$$
$$= G_t^{Q\dagger} + G_t^Q - (E_{T1}-E)^{-1}[G_t^{Q\dagger}Q(H-E)Q + Q(H-E)QG_t^Q + G_t^{Q\dagger}Q(H-E)Q(H-E_{T1})QG_t^Q + Q]. \tag{3.33}$$

It is usual and convenient to choose G_t^Q to be a linear sum of separable terms,

$$G_t^Q = \sum_i a_i |\phi_i\rangle\langle\phi_i| , \tag{3.34}$$

where the ϕ_i are as yet unspecified. If more than one term is retained on the right-hand side, however, the stationary bound on G_v^Q, while still calculable in principle, involves excessive computational effort. That the limitation of (3.34) to a single term is a reasonable choice can be seen from the fact that there exists a separable G_t^Q such that the resulting G_v^Q in (3.33) has the identical effect, when operating on $HP\Psi$, as G^Q itself. In particular, the right-hand side of (3.5), with $f_t = Q\Psi$, is such a separable G_t^Q. Under these circumstances, $\delta G^Q HP\Psi = 0$ and $(G_v - G)HP\Psi = 0$. Accordingly, we write, instead of (3.34), simply

$$G_t^Q = a|\phi\rangle\langle\phi| , \tag{3.35}$$

where, from Sec. III A, we know that ϕ is some approximation to $Q\Psi$. Similarly, the number a might be chosen to be an approximation to λ as defined by (3.8) or, alternatively, a could be carried through as a variational parameter and varied in the final answer to produce the best bound. It will be more convenient, however, to determine a directly from (3.33) via a minimization process. We proceed by substituting (3.35) into (3.33), and write the result as

$$G_v^Q = [a + a^* - maa^*(E_{T1} - E)^{-1}]|\phi\rangle\langle\phi| - (E_{T1} - E)^{-1}[\{a^*|\phi\rangle\langle\phi|\mathcal{K}\} + \{\mathcal{K}|\phi\rangle\langle\phi|a\}] + Q] , \tag{3.36}$$

where we have defined

$$\mathcal{K} \equiv Q(H - E)Q \tag{3.37}$$

and

$$m \equiv \langle\phi|Q(H - E)Q(H - E_{T1})Q|\phi\rangle . \tag{3.38}$$

We next form the diagonal matrix element of G_v^Q with respect to an arbitrary vector χ, and demand that the resulting expression be an extremum with respect to both a and a^*. The resulting values of a and a^* are found to be

$$a = (1/m)(E_{T1} - E - \langle\phi|\mathcal{K}|\chi\rangle/\langle\phi|\chi\rangle) \tag{3.39a}$$

and

$$a^* = (1/m)(E_{T1} - E - \langle\chi|\mathcal{K}|\phi\rangle/\langle\chi|\phi\rangle) . \tag{3.39b}$$

The resulting extremum value of $\langle\chi|G_v^Q|\chi\rangle$ is found to be

$$\langle\chi|G_v^Q|\chi\rangle = m^{-1}(E_{T1} - E)\langle\chi|[1 - \mathcal{K}/(E_{T1} - E)]|\phi\rangle \times \langle\phi|[1 - \mathcal{K}/(E_{T1} - E)]|\chi\rangle - (E_{T1} - E)^{-1}\langle\chi|Q|\chi\rangle . \tag{3.40}$$

From this it is apparent that, with respect to *diagonal* matrix elements, if we choose a and a^* according to (3.39), the operator G_v^Q in (3.36) is equivalent to

$$\mathcal{G}_v^Q = \left(Q - \frac{\mathcal{K}}{E_{T1} - E}\right)|\phi\rangle\frac{E_{T1} - E}{m}\langle\phi|\left(Q - \frac{\mathcal{K}}{E_{T1} - E}\right) - \frac{Q}{E_{T1} - E} , \tag{3.41}$$

and it is this operator which is the more convenient to use in place of G^Q in v of Eqs. (3.4a) and (3.4b). (The unit operator has been replaced by Q in (3.41) as a reminder that G_t^Q—and therefore ϕ—are in Q space.) When this is done we see that, in addition to V_{00}, there arises another local term

$$\hat{V} = -(E_{T1} - E)^{-1}(\psi_{T0}, VQV\psi_{T0}) , \tag{3.42}$$

which may be bounded without difficulty. The nonlocal term must be handled as before. We define a new modified static equation, with $V_{00}^{(-)}$ replaced by $V_{00}^{(-)} + \hat{V}^{(-)}$, and determine the corresponding solution $\hat{u}_s$, the associated phase shift $\hat{\eta}_s$, and Green's function $\hat{G}_s$. The desired stationary upper bound on $\tan\hat{\eta}$ is now obtained from the two-potential formula, Eq. (3.14), with λ replaced by $(E_{T1} - E)/m$, and f_t replaced by

$$(1 - \mathcal{K}/(E_{T1} - E))\phi .$$

The resulting matrix elements in that expression will either be known, or else will consist of matrix elements involving ψ_{T0} of the types considered previously. These must then be replaced by the appropriate upper or lower stationary bounds so as to preserve in this case the *upper* bound on $\tan\hat{\eta}$.

We conclude this section with two remarks. We first note that both the stationary upper and lower bounds we have derived are free of any of the "spurious" singularities[17,21] that can occur in connection with variational principles, since all of the various types of trial functions that occur are derivable from well-defined minimum principles. Second, the trial function Ψ_t calculated in the course of obtaining these stationary bounds is itself a stationary approximation to Ψ.[22] Thus Ψ_t so determined may be useful in other types of calculations. Having analyzed the scattering of a positron by a particular atom at a particular energy, the Ψ_t determined in the course of a scattering analysis which ignores annihilation could be used to obtain a variational estimate of the annihilation-

rate parameter for a positron of that energy on that atom.

IV. DISCUSSION

We now turn to the questions that are raised by the fact the monotonicity theorem implies relationships about the eigenphase shifts rather than about elements of the K matrix. As mentioned in the Introduction, such matters are in a large degree extraneous to our principal concern in this paper, which is how to extend previous work on scattering parameter bounds, which are calculable only when the target wave functions are known precisely, to cases where such precise information about the target is lacking. These questions arise in the earlier work in essentially the same way as they do in the present work. Acordingly, the material of the present section is largely a brief summary of considerations studied elsewhere. However, many of those considerations were presented at a time when only one stationary bound was available; the availability of *both* stationary bounds changes the emphasis somewhat and enables one to proceed with far greater confidence.

We begin by reviewing the steps leading to the stationary bounds of Sec. III. To simplify the discussion, we assume that only one channel is open. Both the lower and upper stationary bounds obtained in Sec. III are arrived at in two steps. In the first step, we replace the exact optical-model potential by stationary bounds. The phase shift $\tilde{\eta}$ ($\hat{\eta}$) associated with the modified equation is a stationary lower (upper) bound on the true phase shift η. The bound is a formal one, because we do not know the modified potential exactly. In the second step, the two-potential formula is used to obtain a stationary lower (upper) bound on $\tan\tilde{\eta}$ ($\tan\hat{\eta}$). It is clear, however, that these bounds will represent rigorous bounds on $\tan\eta$ itself only if the calculation is sufficiently accurate so that $\tilde{\eta}$ and $\hat{\eta}$ lie on the same branch as η. This question has been discussed in detail elsewhere[4,7]; the basic difficulty is that $\tilde{\eta}<\eta<\hat{\eta}$ does not, in general, imply that $\tan\tilde{\eta}<\tan\eta<\tan\hat{\eta}$.

The fundamental question, accordingly, in any practical calculation, is how one can be assured that the calculation is "sufficiently accurate." The answer is that a level of sufficient accuracy can reasonably be assumed to have been reached once the results exhibit stability with respect to small improvements in the wave function. If such an improvement, for example, produces a slightly increased value of $\tan\tilde{\eta}$, it is possible that $\tilde{\eta}$ has increased by a value slightly less than a multiple of π, but it is more likely that $\hat{\eta}$ has increased slightly, and it is *highly* unlikely that the value of $\tan\tilde{\eta}$ would continue to show small increases under a sequence of such improvements in the wave function unless $\tilde{\eta}$ did indeed lie on the correct branch. The salient point is that, as a practical matter, it will almost always be apparent whether or not the condition of stability has been reached. The fact that both upper *and* lower bounds are available will also be of considerable help. In terms of the present paper, where the target functions are imprecisely known, we do not know $\tan\tilde{\eta}$ or $\tan\hat{\eta}$ exactly; if we obtain *both* bounds on both $\tan\tilde{\eta}$ *and* $\tan\hat{\eta}$ (for either of the two tangents, the extra effort required to obtain the other bound once one of the bounds has been obtained is almost nil) then the information, with regard to stability of the solution, will be essentially the same as if we had the exact values of both of these (inexact) quantities. Ultimately, of course, this means that we are formally giving up rigor, but the results can nevertheless play almost as useful a role as if they were rigorous. In particular, the most useful characteristic of rigorous bounds—namely, that they provide an unequivocal means for systematically improving the trial functions—is retained. It might also be remarked that we are, in a sense, giving up rigor by choice rather than necessity. For any of the systems to which the results of this paper are applicable (but not for electron-atom scattering), one could keep track of which branch the phase shift was on by replacing V in the true problem by μV, and requiring that the corresponding phase shift $\eta(\mu)$ vary from 0 to η as μ varied from 0 to unity. The calculational price that one would pay for this, however, is exorbitant, since a series of calculations for intermediate values of μ would have to be performed. Another tactic would be to study the positivity, not of $Q(H-E)Q$ as was done earlier in the text, but of $Q(H+HG^{P}H-E)Q$. This would result in a bound directly on $\tan\eta$ rather than η,[6] but here again the computational difficulties render this approach impractical.

The reader is referred to Refs. 4, 6, and 7 for a more detailed analysis of these questions. We would, however, like to make one last remark, namely, that one can often estimate the numerical accuracy of a calculation performed in a way guaranteed to provide a rigorous stationary bound.[23] Thus, if $\tilde{\eta}$ is expected to increase, but decreases in the third digit, one can be reasonably certain that $\tilde{\eta}$ is only accurate to two significant digits. This result proved useful in the past[23] in the analysis of low-energy scattering calculations of e^{+} and e^{-} on a target with known ψ_T, namely hydrogen, and could be applied to, say, low-energy–e^{+}-helium scattering calculations if performed along the lines suggested in the present paper.

APPENDIX A: CONSTRUCTION OF THE MATRIX $\underline{U}$ FOR AN ARBITRARY NUMBER OF CHANNELS

Suppose we wish to construct $\underline{U} \equiv \underline{U}^{(M+1)}$ for $M+1$ channels, an approximation to $\underline{V}^{(M+1)}$. As a first step one computes all of the functions $V_{ij}^{(\pm)} = V_{ji}^{(\pm)*}$ [defined below Eq. (2.12)]. Then all of the second-order functions

$$v_{ij} \equiv V_{ij}^{(+)} - V_{ij}^{(-)} \tag{A1}$$

are known. The functions

$$\delta^{+} V_{ij} \equiv V_{ij}^{(+)} - V_{ij} \tag{A2}$$

are known to be second order, but are otherwise unknown. Similarly

$$\delta^{-} V_{ij} \equiv V_{ij}^{(-)} - V_{ij} \tag{A3}$$

are second-order unknown functions. We define $\delta V_{ij} = U_{ij} - V_{ij}$.

Next, suppose that the M channel matrix $\underline{U}^{(M)}$ has been constructed. Consider the $(M+1) \times (M+1)$ matrix

$$\underline{U}^{(M+1)} = \left[\begin{array}{c|c} \underline{U}^{(M)} & \begin{matrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \end{matrix} \\ \hline 0 \;\; 0 \;\; \cdots & V_{MM}^{(+)} \end{array}\right] + \left[\begin{array}{ccc|c} u_{00} & & & U_{0M} \\ & u_{11} & & U_{1M} \\ & & \ddots & \cdot \\ & & & \cdot \\ \hline U_{M0} & U_{M1} & \cdots & u_{MM} \end{array}\right]$$

Since we want $\underline{U}^{(M+1)}$ to be Hermitian and a variational approximation to $\underline{V}^{(M+1)}$, we must choose $U_{Mi} = U_{iM}^{*}$, where the U_{Mi} are variational approximations to the V_{Mi}, and the u_{ii} must be second-order quantities. Further, we want

$$\underline{U}^{(M+1)} - \underline{V}^{(M+1)} = \left[\begin{array}{c|c} \underline{U}^{(M)} - \underline{V}^{(M)} & \begin{matrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \end{matrix} \\ \hline 0 \;\; 0 \;\; \cdots & \delta V_{MM} \end{array}\right] + \left[\begin{array}{ccc|c} u_{00} & & & \delta V_{0M} \\ & u_{11} & & \delta V_{1M} \\ & & \ddots & \cdot \\ & & & \cdot \\ \hline \delta V_{M0} & \delta V_{M1} & \cdots & u_{MM} \end{array}\right]$$

to be positive definite. The first matrix on the right-hand-side is clearly positive definite, and a sufficient condition for $\underline{U}^{(M+1)} - \underline{V}^{(M+1)}$ to be positive definite is therefore that the second matrix on the right-hand side be positive definite. This will be the case if the u_{ii}'s are positive,[24] and if its determinant is positive, that is, if

$$\left(\prod_{i=0}^{M-1} u_{ii}\right)\left(u_{MM} - \sum_{j=0}^{M-1} \frac{|\delta V_{jM}|^2}{u_{jj}}\right) \geq 0.$$

Since the product factor is positive, the condition is that the quantity in the second parentheses be positive, that is,

$$u_{MM} \geq \sum_{j=0}^{M-1} \frac{|\delta V_{jM}|^2}{u_{jj}}.$$

This will certainly be the case if we choose the u_{jj}, for $j=0$ to M, such that

$$u_{MM} = \sum_{j=0}^{M-1} \frac{|v_{jM}|^2}{u_{jj}}. \tag{A4}$$

If we choose $u_{jj} = u$ for $j=0$ to M, u can be chosen to be

$$u = \left(\sum_{j=0}^{M-1} |v_{jM}|^2\right)^{1/2}, \tag{A5}$$

and U_{iM}, with $i \neq M$, chosen to be $V_{iM}^{(+)}$. This represents one solution to the problem.

The above constructions reduce for $M=1$ to the 2×2 case considered in Sec. II. Thus, with the $v_{jM} = v_{j1}$, Eq. (A5) gives $u = |v_{01}|$, which corresponds to (2.14b) with $\alpha = 1$. If we do not set $u_{11} = u_{00} = u$, (A4) reads

$$u_{00} u_{11} = |v_{01}|^2,$$

which is satisfied if $u_{00} = \alpha |v_{01}|$, $u_{11} = |v_{11}|/\alpha$, $\alpha > 0$, and this corresponds exactly to (2.14b). In the general case, we can introduce a different variational parameter for each of the u_{ii} by choosing $u_{ii} = \alpha_i u$ [there will be a total of $\frac{1}{2}(M+1)(M+2) - 1$ such α_i's], but it appears doubtful if the advantages of such a procedure outweigh the disadvantages entailed by the extra computational labor involved.

In summary, the matrix $\underline{U}$ we found is given as follows [where we write our results now in terms of the M-channel case rather than the $(M+1)$-channel case]:

$$\begin{aligned} U_{ij} &= V_{ij}^{(+)}, \quad i \neq j \\ U_{ii} &= V_{ii}^{(+)} + \sum_{L=1}^{M-1} \left(\sum_{k=0}^{L-1} |v_{kL}|^2\right)^{1/2}. \end{aligned} \tag{A6}$$

Note that Eqs. (A6) imply that each element of $\underline{U} - \underline{V}$ is a second-order quantity.

APPENDIX B: POSITIVITY OF $Q_t(H_T-E)Q_t$

The difficulties in establishing the positive definiteness of $Q(H_T-E)Q$, (when the operator is, in fact, positive definite), are largely a consequence of the fact that Q is not known. As was mentioned in Sec. III B, it is rather simple to determine conditions under which $Q_t(H_T-E)Q_t>0$, where $E_{T0}\leq E\leq E_{T1}$. Without loss of generality, we may limit the discussion to an examination of matrix elements of the form

$$(\chi,(H_T-E)\chi), \tag{B1}$$

where χ and ψ_{T0t} are orthogonal (so that χ is in Q_t space) and normalized. It is convenient to introduce the expansions

$$\psi_{T0t}=\sum_i c_i\psi_{Ti} \tag{B2}$$

and

$$\chi=\sum_i b_i\psi_{Ti}, \tag{B3}$$

where the subscript ranges from 0 to ∞, so that

$$\sum_i c_i^* b_i=0,\quad \sum_i |c_i|^2=\sum_i |b_i|^2=1. \tag{B4}$$

We wish to ensure that matrix elements of the form (B1) will be positive, that is, that

$$\sum_i |b_i|^2(E_{Ti}-E)\geq 0, \tag{B5}$$

or

$$|b_0|^2(E-E_{T0})\leq \sum_i{}' |b_i|^2(E_{Ti}-E). \tag{B6}$$

The subscript in the primed sum ranges from 1 to ∞, and, noting that $E_{T1}-E\leq E_{Ti}-E$ for that range of i, it follows that (B6) will be satisfied if

$$|b_0|^2(E-E_{T0})\leq (E_{T1}-E)\sum_i{}' |b_i|^2=(E_{T1}-E)(1-|b_0|^2)$$

is satisfied, that is, if

$$|b_0|^2\leq (E_{T1}-E)/(E_{T1}-E_{T0}). \tag{B7}$$

Moreover, it follows easily[25] from (B4) that

$$|b_0|^2\leq 1-|c_0|^2. \tag{B8}$$

Equation (B7) will therefore be satisfied if the right-hand side of (B8) is less than the right-hand side of (B7), that is, if

$$|c_0|^2\geq (E-E_{T0})/(E_{T1}-E_{T0}). \tag{B9}$$

The Eckart bound[26] on $|c_0|^2$ gives

$$|c_0|^2\geq (E_{T1}-E_{T0t})/(E_{T1}-E_{T0}). \tag{B10}$$

Equation (B9) will be satisfied if the right-hand side of (B10) is greater than the right-hand side of (B9), that is, if

$$E_{T0t}\leq E_{T1}-(E-E_{T0}). \tag{B11}$$

Equation (B11) is a condition which guarantees the positive definiteness of $Q_t(H_T-E)Q_t$.

---

*Work supported by the U. S. Army Research Office, Durham, Grant No. DA-ARO-D-31-124-72-G92, and by the Office of Naval Research, Contract No. N00014-67-A-0467-0007.

†Supported in part by funds from the National Science Foundation under Grant No. GU-3186.

‡Work supported by the National Science Foundation.

[1]L. Spruch and L. Rosenberg, Phys. Rev. 117, 1095 (1960).

[2]R. Blau, L. Rosenberg, and L. Spruch, Phys. Rev. A 10, 2246 (1974).

[3]R. Blau, L. Rosenberg, and L. Spruch, Phys. Rev. A 11, 200 (1975).

[4]Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. 134, B397 (1964).

[5]See also, R. Blau, A. R. P. Rau, and L. Spruch, Phys. Rev. A 8, 131 (1973).

[6]See, for example, Y. Hahn and L. Spruch, Phys. Rev. 153, 1159 (1967).

[7]See also, Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. 130, 138 (1963).

[8]In principle, since the target energies are not known precisely, one must minimize the phase shifts over *ranges* of the $M-1$ variables $E_i'=E-E_{Ti}$, $i=1,2,\ldots,M-1$, if one is to maintain a rigorous result. (One may consider that one of the E_i', say, E_k', is given. Then bounds on E_{Tk} determine a range for E, and these, together with bounds on the other E_{Ti}, determine ranges for the other E_i'.) In practice, however, it is anticipated that the bounds on the E_{Ti}'s will be sufficiently accurate that the change in the phase shifts over these ranges will be negligible, thus rendering such a minimization process unnecessary.

[9]See, for example, E. F. Beckenbach and R. Bellman, *Inequalities* (Springer, Berlin, 1965), Chap. 2. The proof is given for symmetric matrices but the extension to Hermitian matrices is straightforward.

[10]H. Feshbach, Ann. Phys. (N.Y.) 5, 337 (1958); 19, 287 (1962).

[11]If there are $M>1$ open excitation channels, we will have, instead of V_{00}, the $M\times M$ matrix $\underline{V}=\|V_{ij}\|$. This can then be replaced by the matrix $\underline{U}$, constructed as per Sec. II, in the M coupled equations which replace (3.4a).

[12]L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. 118, 184 (1960).

[13]M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964), p. 202.

[14]C. Schwartz, Ann. Phys. (N.Y.) 2, 156 (1959); 2, 170 (1959); A. Dalgarno and A. L. Stewart, Proc. R. Soc.

A 257, 534 (1960); J. C. Y. Chen and A. Dalgarno, Proc. R. Soc. 85, 399 (1965); L. M. Delves, Proc. Phys. Soc. Lond. 92, 55 (1967).

[15]J. O. Hirschfelder, W. B. Brown, and S. T. Epstein, Adv. Quantum Chem. 1, 255 (1964).

[16]See also, E. Gerjuoy, A. R. P. Rau, and L. Spruch, Phys. Rev. A 8, 662 (1973).

[17]E. Gerjuoy, A. R. P. Rau, L. Rosenberg, and L. Spruch, Phys. Rev. A 9, 108 (1974).

[18]A variational principle for (x, y) in the form (3.29), where x and y are related by the Hermitian operator O according to the relationship $Ox = y$ is given by N. Marcuvitz [*Recent Developments in the Theory of Wave Propagation* (New York University, Institute for Mathematics and Mechanics, New York, 1949), Sec. III D]. In our case, where $O = Q_t(H - E)Q_t$ is of well-defined sign, the sign of the error is known, and the variational principle is also an extremum principle. See L. Spruch, in *Lectures in Theoretical Physics, Boulder, 1961*, edited by W. E. Britten, W. B. Downs, and J. Downs (Wiley, New York, 1962), Vol. 4, p. 161. The use of this type of functional in obtaining a subsidiary minimum principle for the trial auxiliary function L_{T0t} is given in Ref. 17. See also, S. Aranoff and J. Percus, Phys. Rev. 166, 1255 (1968). The extremum principle, for O positive definite, has been known to mathematicians for a very long time.

[19]P. G. Burke and J. A. Taylor, Proc. Phys. Soc. 88, 549 (1966).

[20]R. Sugar and R. Blankenbecler, Phys. Rev. 136, B472 (1964); J. Carew and L. Rosenberg, Phys. Rev. C 5, 658 (1972).

[21]C. Schwartz, Ann. Phys. (N. Y.) 16, 36 (1961).

[22]It is clear that the approximation to $P\Psi$ obtained in Sec. III A is a stationary one, since every step in the derivation involves only second-order or higher error terms. Furthermore, we may obtain a stationary approximation to $Q\Psi$ via Eq. (3.26), since, as we have seen, the right-hand side of (3.5) is a stationary bound on G^Q. Thus a stationary approximation to $\Psi = P\Psi + Q\Psi$ can be determined.

[23]Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. 128, 932 (1962).

[24]The theorem on positive-definite matrices (p. 59 of Ref. 9) holds for non-negative matrices only as a limiting case of positive-definite matrices, and not in general. For this reason, we cannot choose the u_{ii}'s equal to zero at the outset. The u_{ii}'s in fact, must satisfy the inequality above Eq. (A4), and can approach zero only as the δV_{jM}'s approach zero. In this limit, of course, $\underline{U} - \underline{V}$ equals the zero matrix, and the bound becomes an equality.

[25]E. Gerjuoy, L. Rosenberg, and L. Spruch, J. Math. Phys. 16, 455 (1975).

[26]C. Eckart, Phys. Rev. 36, 878 (1930).