Lower Bounds on the Inverse Reactance Matrix*

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The spectrum of the closed-channel Hamiltonian $\mathcal{H}$ in the multichannel scattering problem is bounded from below and by construction is discrete in the energy region below the threshold for new channels. This property has been applied previously to derive a minimum principle which provides an upper bound on the inverse reactance matrix. The discreteness of the spectrum of $\mathcal{H}$ in the region below the threshold for new channels is further exploited here to derive lower bounds. Forms linear as well as quadratic in $\mathcal{H}$ are obtained and their applicability discussed. Extensive use of the Unsöld approximation and the closure properties of the states generated by the various operators is necessary in order to reduce the inequalities to manageable forms. An iterative method to treat the energy shift operator is discussed, and the convergence of the iteration series and its connection to the subtraction terms in the minimum principle are discussed in detail.

I. INTRODUCTION

ONE of the unsatisfactory features of the usual variational principles in scattering problems is that they do not automatically give a bound on scattering parameters, contrary to the case with the Ritz method for the bound-state problem. Thus it is not always guaranteed that as additional parameters are introduced into the variational calculation the result will always improve.[1,2]

The minimum principle derived previously[3] provides one such bound, an upper bound on the inverse reactance matrix, or on $\cot\eta$ for the case of single-channel scattering. The derivation was carried out by first converting the original scattering problem with the total Hamiltonian H into an "associated" bound-state problem. That is, when all the open channels of the scattering system at fixed energy E are projected out, the resulting closed-channel Hamiltonian $\mathcal{H}$ has an energy spectrum which is bounded from below and *discrete* in the energy region below the threshold for new channels, essentially analogous to the spectrum of the bound states. A variational principle can then be set up and one obtains, for a given scattering energy, a bound on the scattering parameters. Unlike the case of the usual variational principles of the Kohn, Hulthén, and Schwinger types, the bound converges monotonically to the correct value from above as more variational parameters are added.

However, it is often difficult to estimate the accuracy of the bound thus obtained and even a crude opposite bound may be very useful. Unfortunately, the operators one deals with are usually bounded only from *below*, and this makes the derivation of the opposite bound very cumbersome; one is almost always forced to construct[4] operators such as H^2 or to divide the original H into two or more terms each with specified properties.[5] Many such methods are known for bound-state problems, and the similarity between the spectrum of $\mathcal{H}$ and that of the operator H for the bound-state problem allows us to apply them to obtain lower bounds on the inverse-reactance matrix.

One feature peculiar to this problem is that, unlike the upper bound, the lower bound requires the treatment of the *entire* spectrum without truncation. Therefore, an extensive use of the Unsöld approximation and of closure properties is necessary in order to preserve the rigor of the bounds and yet put the resulting bounds in manageable forms for application.

Our main results are the quadratic bounds given by (3.17) and (3.21) and the linear bound (4.39), with $Q\Psi_k$ given by (4.37) and the subsequent modification by iterations involving (4.38).

II. FORMALISM-UPPER BOUNDS

In order to introduce the notation and also to improve on the minimum principle in some points, a brief review of the previous result[3] will be given. The projection operators[6] P and Q are defined such that P projects onto *all* the open channels for a given fixed total energy E. The operator P can further contain an arbitrary number of closed-channel states, but we do not consider this possibility here nor the possible simplification which results when E reaches the threshold for new channels. These can be incorporated into the formalism in a simple way. The operator Q projects onto the closed channels only, and hence

$$P+Q=1\,,$$
$$P^2=P\,,\quad Q^2=Q\,,\quad PQ=0\,. \tag{2.1}$$

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[1] For a review of the problem, see for example L. Spruch, in *Lectures in Theoretical Physics, Boulder, Colorado, 1961* (Interscience Publishers, Inc., New York, 1961), Vol. 4.

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[6] H. Feshbach, Ann. Phys. (N. Y.) **19**, 287 (1962).

The Schrödinger equation,

$$(H-E)\Psi=0, \tag{2.2}$$

can be written as a set of two coupled equations

$$P(H-E)P\Psi=-PHQ\Psi, \tag{2.3}$$

$$Q(H-E)Q\Psi=-QHP\Psi. \tag{2.4}$$

Equations (2.3) and (2.4) can be solved formally for $P\Psi$ and $Q\Psi$ as

$$P\Psi=P\Psi^P+PG^PPHQ\Psi, \tag{2.5}$$

$$Q\Psi=QG^QQHP\Psi, \tag{2.6}$$

where

$$P(H-E)P\Psi^P=0, \tag{2.7}$$

$$P(H-E)PG^P=-P, \tag{2.8}$$

and

$$Q(H-E)QG^Q=-Q. \tag{2.9}$$

The functions $P\Psi^P$, $P\Psi$, and PG^PP satisfy the usual standing-wave boundary conditions, while $Q\Psi$ vanishes asymptotically faster than the inverse of the distance coordinates corresponding to each closed channel. Substitution of (2.6) and (2.5) into the right-hand sides of Eqs. (2.3) and (2.4), respectively, formally uncouples the equations. The resulting equations are

$$P(H+HG^QH-E)P\Psi=0, \tag{2.10}$$

$$Q(H+HG^PH-E)Q\Psi=-QHP\Psi^P. \tag{2.11}$$

Equation (2.10) was the basis for discussion of the various upper bounds on the inverse reactance matrices obtained by the close-coupling approximations,[6a] while Eq. (2.11) can be solved variationally for $Q\Psi$ giving rise to the minimum principle.[3] For a trial function $Q\Psi_t$, one has

$$\begin{aligned}\lambda\leq\lambda_U&=\lambda^P+2(Q\Psi_t,QHP\Psi^P)+(Q\Psi_t,[\mathcal{K}-E]Q\Psi_t)\\&\quad+\sum_{n=1}^{N^Q}\frac{|(Q\Phi_{nt}{}^Q,[(\mathcal{K}-E)Q\Psi_t+QHP\Psi^P])|^2}{E-\mathcal{E}_{nt}{}^Q},\end{aligned} \tag{2.12}$$

where

$$\begin{aligned}\lambda&=\mathbf{a}\cdot\mathbf{K}^{-1}\mathbf{a},\\\lambda^P&=\mathbf{a}\cdot(\mathbf{K}^P)^{-1}\mathbf{a},\\\mathcal{K}&=Q(H+HG^PH)Q.\end{aligned} \tag{2.13}$$

$\mathbf{a}$ is an arbitrary constant vector and λ^P corresponds to the parameter obtained from $P\Psi^P$. $Q\Phi_{nt}{}^Q$ are the "bound state" trial functions, which must satisfy

$$(Q\Phi_{nt}{}^Q,\mathcal{K}Q\Phi_{mt}{}^Q)=\mathcal{E}_{nt}{}^Q\cdot\delta_{nm}<E$$

and which approximate the resonant states. The term involving G^P in $\mathcal{K}$ produces a shift in the resonance energies due to the coupling between P channels and Q channels.

From the computational point of view, the minimum principle (2.12) contains the following complications which are not present in the usual Kohn or Hulthén variational methods:

(i) The exact operator P must be constructed. This in turn provides the Q operator which is used to construct explicitly the trial function $Q\Psi_t$. This is often very difficult to do.

(ii) The exact solution $P\Psi^P$ must be calculated from Eq. (2.7). This is not a serious complication as long as the number of open channels in P is small.

(iii) The exact Green's function G^P defined by Eq. (2.8) must be constructed. This is the most serious complication of the minimum principle and can be avoided by an iterative method to be described in Appendix A.

(iv) The subtraction terms in Eq. (2.12) must be evaluated. It has been shown however that for a "good enough" trial function $Q\Psi_t$, these terms are automatically taken into account and that an explicit subtraction may often not be necessary.[3]

A possible way to eliminate the requirement (ii) is discussed in Sec. VI, but we are not able to give a proof, while the requirement (i) is still to be satisfied and this prevents us from applying the minimum principle to the more complicated systems involving more than three particles.

The linearity of (2.12) with respect to the closed-channel operator $\mathcal{K}$ is a great advantage over some of the other methods introduced earlier, even with the complications mentioned above. Unfortunately, such a general linear method as the Ritz principle for the bound state problem does not seem possible for the lower bound on λ. In the next section, the lower bounds involving the $\mathcal{K}^2$ operator will be given, while in Sec. IV, the bounds involving a linear form in $\mathcal{K}$, but only applicable to a very restricted class of problems, will be discussed.

Before studying such bounds, it is of interest for later comparison to cast (2.12) in a modified form, using $\mathcal{E}_{nt}{}^Q$ and $Q\Phi_{nt}{}^Q$ which are obtained by the diagonalization of the energy matrix associated with $\mathcal{K}$. For an $M\times M$ matrix, where M is the number of the trial functions in $Q\Psi_t$, we have, with $M\geqslant N^Q$,

$$\lambda_U=\lambda^P+\sum_{m=1}^{M}\frac{|(Q\Phi_{mt}{}^Q,QHP\Psi^P)|^2}{E-\mathcal{E}_{mt}{}^Q}. \tag{2.14}$$

Note that $\lambda_U\to\lambda$ as $M\to\infty$ and that the truncation of the series in (2.14) is permitted since the mth term in the sum makes a negative contribution if $m>N^Q$. Note also that in this particular representation the subtraction terms are identically zero. As will be shown, such truncation is not allowed for the lower bound; on the contrary the entire series has to be bounded from

[6a] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **128**, 932 (1962); **134**, B397 (1964).

below. This may be the principal reason why the lower bound on λ is usually much harder to obtain.

III. LOWER BOUND—QUADRATIC FORMS

The expressions for the lower bound to be derived in this section involve the $\mathcal{H}^2$ operator and resemble the formulas given by Temple[7] and by Stevenson and Crawford[8] for the bound state problem. There are nontrivial differences in the derivation however. Firstly, unlike the bound state problem, one has here the inhomogeneous Eq. (2.11) with the energy E fixed. Thus the normalization of the wave function $Q\Psi$ is no longer arbitrary. Secondly, the quantity being calculated is $\lambda-\lambda^P$ which involves the Green's function G^Q defined by Eq. (2.9). This means that it is necessary to make subtractions when there are states of $\mathcal{H}$ with the energies $\mathcal{E}_n{}^Q<E$ in the case of the upper bound and caution is also required in the case of the lower bound.

For the moment, we assume that the operator $Q(E-\mathcal{H})Q$ is negative definite. We write Eq. (2.11) in the form

$$(\mathcal{H}-E)Q\Psi=-QHP\Psi^P\equiv-R_0 \tag{3.1}$$

and we introduce

$$(\mathcal{H}-E)Q\Psi_t\equiv-R_{0t}. \tag{3.2}$$

Now consider a positive semidefinite quantity I defined by

$$I\equiv(R_0-R_{0t},\,R_0-R_{0t})\geq 0. \tag{3.3}$$

The functions $Q\Psi$ and $Q\Psi_t$ can be expanded in terms of the set $Q\Phi_n{}^Q$

$$Q\Psi=\sum_n a_nQ\Phi_n{}^Q, \tag{3.4}$$

$$Q\Psi_t=\sum_n a_{nt}Q\Phi_n{}^Q, \tag{3.5}$$

where $Q\Phi_n{}^Q$ are generated by the operator $\mathcal{H}$,

$$\mathcal{H}Q\Phi_n{}^Q=\mathcal{E}_n{}^QQ\Phi_n{}^Q, \tag{3.6}$$

with

$$(Q\Phi_n{}^Q,Q\Phi,_m{}^Q)=\delta_{nm}.$$

The sums in (3.4) and (3.5) include continuum states as well. The quantity I can then be written as

$$I=\sum_n(a_{nt}-a_n)^2(\mathcal{E}_n{}^Q-E)^2, \tag{3.7}$$

which is the starting point for the derivation of lower bounds.

Since we have assumed that $\mathcal{E}_n{}^Q>E$ holds for all n, we obtain

$$\begin{aligned}I&\geq(\mathcal{E}_1{}^Q-E)\sum_n(a_{nt}-a_n)^2(\mathcal{E}_n{}^Q-E)\\&=(\mathcal{E}_1{}^Q-E)\{2(Q\Psi_t,R_0)\\&\qquad+(Q\Psi_t,[\mathcal{H}-E]E\Psi_t)-(Q\Psi,R_0)\}.\end{aligned} \tag{3.8}$$

Thus, if $Q(E-\mathcal{H})Q$ is negative definite, we have the lower and the upper bounds

$$\Delta_L\leq\Delta\leq\Delta_U, \tag{3.9}$$

where

$$\Delta\equiv\lambda-\lambda^P=(Q\Psi,R_0), \tag{3.10}$$

and

$$\Delta_L=\Delta_M-I/(\mathcal{E}_1{}^Q-E), \tag{3.11}$$

$$\begin{aligned}\Delta_U&=\lambda_U-\lambda^P=2(Q\Psi_t,R_0)+(Q\Psi_t,[\mathcal{H}-E]Q\Psi_t),\\&\equiv\Delta_M.\end{aligned} \tag{3.12}$$

A trivial but interesting special case of (3.11) is obtained by putting $Q\Psi_t=0$; we then have

$$\Delta_L{}^{(0)}=(R_0,R_0)/(E-\mathcal{E}_1{}^Q), \tag{3.13}$$

which could also be expected directly from Eq. (2.10)[8a] by applying the Unsöld approximation. That is,

$$\begin{aligned}&(P\Psi^P,PHQ\bar{G}^QQHP\Psi^P)\\&\qquad\geqslant(P\Psi^P,PHQ\delta QHP\Psi^P)/(E-\tilde{\epsilon})\\&\qquad=(R_0,R_0)/(E-\tilde{\epsilon}),\end{aligned}$$

with $Q(\mathcal{H}-E)Q\bar{G}^Q=-Q$ and the constant $\tilde{\epsilon}$ satisfies the inequality $E<\tilde{\epsilon}\leqslant\mathcal{E}_1{}^Q$. Explicitly we have $PHQ\delta QHP=PV^2P-(PVP)^2$, where V is the part of H which does not commute with P. Thus we can define the effective average fluctuation potential[9] due to the virtual excitation of the target to all states included in the Q operator as

$$\langle V\rangle=(PV^2P-(PVP)^2)/(E-\tilde{\epsilon}), \tag{3.14}$$

where $-(E-\tilde{\epsilon})^{-1}$ is the "average energy" of the operator $(\mathcal{H}-EQ)^{-1}$.

For the lower bound defined by the inequality (3.9) and Eq. (3.11) to be rigorous, it is necessary to know the value of $\mathcal{E}_1{}^Q$ exactly or to replace it by its lower bound. However, it is often possible to replace it by an approximate value $\mathcal{E}_{1t}{}^Q$ which may be available from some other means, and still obtain a useful bound, as long as I is sufficiently small and $\mathcal{E}_1{}^Q$ is not too close to E. The form of Δ_L given by (3.11) is the direct analog of the formula given by Temple for the bound state problem.

So far, the question of possible subtractions for Δ_L has not been treated. When one or more bound states of $\mathcal{H}$ lie below E, the expressions (3.11) and (3.12) require modifications. As already shown in (2.12), Δ_U is to be changed to a form

$$\Delta_U=\Delta_M+\sum_{n=1}^{N^Q}\frac{|(Q\Phi_{nt},[\mathcal{H}-E]Q\Psi_t+R_0)|^2}{E-\mathcal{E}_{nt}{}^Q}, \tag{3.15}$$

[7] G. Temple, Proc. Roy. Soc. (London) **A119**, 276 (1928).

[8] A. F. Stevenson and M. F. Crawford, Phys. Rev. **54**, 375 (1938). Also, see the recent application to the He problem by T. Kinoshita, Phys. Rev. **115**, 366 (1959).

[8a] This observation was first made by Professor L. Spruch. See for example, L. Spruch, Lectures given at the Ninth Yugoslavian Summer Meeting of Physicists: Few Nuclear Problems; Hercegnovi, July 1964 (unpublished).

[9] For example, see H. Feshbach, Ann. Rev. Nucl. Sci. **8**, 49 (1958).

while Δ_L is to be modified as

$$\Delta_L=\Delta_M-\frac{I}{\mathcal{E}_{N^Q+1}{}^Q-E}+\sum_{n=1}^{N^Q}\frac{|(Q\Phi_n,[\mathcal{H}-E]Q\Psi_t+R_0)|^2}{E-\mathcal{E}_n{}^Q}\times\frac{(\mathcal{E}_{N^Q+1}{}^Q-\mathcal{E}_n{}^Q)}{(\mathcal{E}_{N^Q+1}{}^Q-E)},\quad(3.16)$$

with

$$\mathcal{E}_n{}^Q<E<\mathcal{E}_{N^Q+1}{}^Q,\quad n=1,2,\cdots,N^Q.\quad(3.17)$$

We note that, in Eq. (3.16), the quantities $\mathcal{E}_n{}^Q$, $\mathcal{E}_{N^Q+1}{}^Q$, and $Q\Phi_n$ are all *exact*, and therefore (3.16) is not very useful as it stands. However, again these quantities may be replaced either by their appropriate upper and lower bounds resulting in the rigorous bound, or by their approximate values and one obtains a useful estimate of the bound. We note that the subtraction terms are positive and thus can be neglected entirely.

As the total energy E approaches one of the eigenvalues of the operator $\mathcal{H}$, (3.16) becomes impractical due to the singularity in the energy denominator. To avoid such singularities, an alternate expression for Δ_L can be derived, which may be more adequate for the case when E is very close to the resonance energy.

Consider the positive semidefinite quantity I_c defined by

$$I_c\equiv(R_0-cR_{0t},\,R_0-cR_{0t})=\sum_n(a_n-ca_{nt})^2(\mathcal{E}_n{}^Q-E)^2\geq 0,\quad(3.18)$$

where c is a parameter to be adjusted to make I_c a minimum for a given R_{0t}. Multiplying both sides of (3.18) by $(Q\Psi,Q\Psi)=\sum_n a_n{}^2\neq 1$, and rearranging the right-hand side, we get

$$I_c(Q\Psi,Q\Psi)\geq[-c(Q\Psi_t,R_0)+(Q\Psi,R_0)]^2.\quad(3.19)$$

If the variational parameter c is chosen such that

$$c\geqslant(R_0,Q\Psi_t)/(Q\Psi_t,[E-\mathcal{H}]Q\Psi_t)>0,\quad(3.20)$$

then Δ_L becomes

$$\Delta_L=c(Q\Psi_t,R_0)-I_c{}^{1/2}(Q\Psi,Q\Psi)^{1/2}.\quad(3.21)$$

This is the desired bound which does not involve the singular denominator. Of course the factor $(Q\Psi,Q\Psi)^{1/2}$ is not known and (3.21) as it stands cannot be used to obtain a rigorous lower bound. Again replacing $(Q\Psi,Q\Psi)^{1/2}$ by $(Q\Psi_t,Q\Psi_t)^{1/2}$, it is possible to obtain an estimate on Δ_L.

The lower bound (3.21) is an analog of the form given by Stevenson and Crawford for the bound state problem. Contrary to the energy eigenvalue problem, the normalization of the wave function $Q\Psi$ is *not* arbitrary in the present scattering problem. This peculiarity originated from the inhomogeneity of the Q equation given by (2.11). Owing to the square root of I_c appearing in the right-hand side of (3.21), it is expected in general that (3.21) will be a poorer lower bound than the form (3.11), except when the energy E approaches one of the eigenvalues of $\mathcal{H}$. On the other hand one may be able to iterate on c and $Q\Psi_t$ and improve on Δ_L somewhat.

The lower bounds (3.11) and (3.21) both involve a quadratic operator in $\mathcal{H}$ through the expressions for I and I_c, and hence there is not much advantage over, for example, the Kato method[4] which involves H^2. However, here the upper bound is linear in $\mathcal{H}$ and thus Δ_L needs to be evaluated once as soon as a fairly accurate $Q\Psi_t$ is obtained from the Δ_U calculation. It is not necessary to solve the "associated potential strength eigenvalue problem" as in Kato's method.

In the next section, still another method of obtaining the lower bound will be discussed which involves the operator $\mathcal{H}$ only linearly. Before leaving this section, we recast the form of I given by (3.3) in a form which does not involve the Green's function G^P. For this purpose we use the result of Appendix A. There we have defined the function $P\tilde{\Psi}_t$ as the *exact* solution of the equation

$$P(H-E)P\tilde{\Psi}_t=-PHQ\Psi_t,\quad(3.22)$$

for a given $Q\Psi_t$. Using (3.22) and (3.1), (3.2), it is straightforward algebra to calculate R_0-R_{0t}; we get

$$R_0-R_{0t}=Q(H-E)Q\Psi_t+QHP\tilde{\Psi}_t.\quad(3.23)$$

Thus we have an alternative form for I,

$$I=(Q(H-E)\tilde{\Psi}_t,\,Q(H-E)\tilde{\Psi}_t)\quad(3.24)$$

with

$$\tilde{\Psi}_t\equiv P\tilde{\Psi}_t+Q\Psi_t,\quad(3.25)$$

which is the desired result. The Green's function G^P does not appear explicitly in (3.24), but is only contained implicitly in the scattering function $P\tilde{\Psi}_t$. A similar expression can also be obtained for I_c.

IV. LOWER BOUND—LINEAR FORMS

It has been discussed so far that, for a real symmetric operator $\mathcal{H}$ whose spectrum is bounded from below and discrete up to the threshold, we have a variational principle which provides an upper bound on the inverse reactance matrix, and also a method to estimate its accuracy by obtaining a lower bound which involves the operator $\mathcal{H}$ in a quadratic form. The method to be studied in the present section provides a lower bound which involves $\mathcal{H}$ only *linearly*. It is a natural extension of the method used by Bazley[5] for the case of bound state problems.

For the present purpose, the closed-channel Hamiltonian $\mathcal{H}$ is written in the form

$$\mathcal{H}=\mathcal{H}_0+\mathcal{V}+\mathcal{U}=\mathcal{H}_v+\mathcal{U},\quad(4.1)$$

where

$$\mathcal{V}=QVQ,$$
$$\mathcal{U}=QHPG^PPHQ,$$
$$\mathcal{H}_v=QHQ.$$

It is essential that everything about the operator $\mathcal{H}_0$ is known, its energy eigenvalues and eigenfunctions, and that the interaction operator $\mathcal{V}$ is positive definite. For most of the discussion in this section, we assume that the effect of $\mathcal{U}$ on the spectrum of $\mathcal{H}$ is small; details of the treatment of $\mathcal{U}$ will be given in part C. Of course it is not unique as to which part of $\mathcal{H}$ should be in $\mathcal{V}$ and which in $\mathcal{H}_0$ as long as the above requirements are satisfied. On the other hand, there are very few physically realistic problems which can be made to satisfy the requirements and this seriously limits the applicability of the method.

The method is given in three steps. Firstly, the operator $\mathcal{H}_0$ is treated alone to obtain bounds on Δ, assuming that $\mathcal{U}$ is negligible and since $\mathcal{V}$ is by definition positive definite. Secondly, the effect of $\mathcal{V}$ is introduced step by step, by constructing the intermediate operators $\mathcal{H}^{(k)}$, which approach the operator $\mathcal{H}_v=\mathcal{H}_0+\mathcal{V}$ uniformly from *below* as $k\rightarrow\infty$. By solving the $\mathcal{H}^{(k)}$ problem in such a way as to preserve the bound on Δ, one finally obtains an improved rigorous bound, again neglecting the effect of the shift potential $\mathcal{U}$. Finally, an iterative method to take into account the effect of $\mathcal{U}$ is discussed.

Before going into the details of the procedure, it is necessary to stress one important difference between applying the intermediate operator method to the bound state problem and to the scattering problem. In the case of the bound state problem, the problem involving $H^{(k)}$ is solved for some low-lying states of H_0 and the rest of the states of H_0 can be ignored, without destroying the rigor of the lower bounds thus obtained on the energy eigenvalues of H. This is not however the case with the scattering problem, where the Green's function corresponding to the operator $(\mathcal{H}^{(k)}-QE)$ is required with its *full* spectrum. Rigorous lower bounds on the *entire* spectrum of $\mathcal{H}^{(k)}$ are necessary in order to preserve the rigor of the bounds.

A. Base Problem

When the energy shift operator $\mathcal{U}=QHG^PHQ$ is neglected for the moment, Eq. (3.1) reduces to

$$(\mathcal{H}_0+\mathcal{V}-E)Q\Psi=-R_0\,, \tag{4.2}$$

where $\mathcal{V}$ is a positive definite operator. The operator $\mathcal{H}_0$ generates a complete set of states in Q space

$$\mathcal{H}_0Q\Phi_n{}^{(0)}=\mathcal{E}_n{}^{(0)}Q\Phi_n{}^{(0)}\,, \tag{4.3}$$

with

$$(Q\Phi_n{}^{(0)},Q\Phi_m{}^{(0)})=\delta_{nm}$$
$$\mathcal{E}_1{}^{(0)}\leq\mathcal{E}_2{}^{(0)}\leq\cdots.$$

It is assumed that the operator $\mathcal{H}_0$ is so simple that the eigenvalues $\mathcal{E}_n{}^{(0)}$ and the eigenfunctions $Q\Phi_n{}^{(0)}$ can be calculated exactly. The separability of $\mathcal{H}_v=\mathcal{H}_0+\mathcal{V}$ to meet the above requirements is essential for the present method to be applicable.

We consider the equation

$$(\mathcal{H}_0-E)Q\Psi^{(0)}=-R_0\,, \tag{4.4}$$

which gives

$$\Delta^{(0)}\equiv(Q\Psi^{(0)},R_0)=\sum_{n=1}^{\infty}(R_0,Q\Phi_n{}^{(0)})^2/(E-\mathcal{E}_n{}^{(0)})\,. \tag{4.5}$$

If the scattering energy E is such that $\mathcal{E}_n{}^{(0)}>E$ for all n, the Unsöld approximation and the completeness of the set $\{Q\Phi_n{}^{(0)}\}$ lead to the bound

$$\Delta^{(0)}\geq\Delta_N{}^{(0)}$$
$$=\frac{1}{E-\mathcal{E}_N{}^{(0)}}\left[(R_0,R_0)-\sum_{n=1}^{N-1}(R_0,Q\Phi_n{}^{(0)})^2\times\frac{(\mathcal{E}_N{}^{(0)}-\mathcal{E}_n{}^{(0)})}{(E-\mathcal{E}_n{}^{(0)})}\right], \tag{4.6}$$

where N is arbitrary. The bound is improved as N is increased. The inequality (4.6) is not valid when there are $N^{Q(0)}$ states of $\mathcal{H}_0$ which lie below E, i.e., $\mathcal{E}_n{}^{(0)}<E$ for $n=1,2,\cdots,N^{Q(0)}$, since for these states the inequality sign should be reversed. The modified form is possible but not useful as it stands since it requires information on the spectrum of $\mathcal{H}_v$ which will be discussed next [see Eq. (4.32)].

B. Intermediate Problems

If the effect of the positive definite operator $\mathcal{V}$ is small, then all the eigenvalues of $\mathcal{H}_0$ are shifted down by roughly the amounts $(Q\Phi_n{}^{(0)},\mathcal{V}Q\Phi_n{}^{(0)})$ and the quantity Δ by roughly

$$\sum_{nm}\frac{(R_0,Q\Phi_n{}^{(0)})(Q\Phi_n{}^{(0)},\mathcal{V}Q\Phi_m{}^{(0)})(Q\Phi_m{}^{(0)},R_0)}{(E-\mathcal{E}_n{}^{(0)})(E-\mathcal{E}_m{}^{(0)})}\,. \tag{4.7}$$

However, we are interested in developing a method which takes into account the effect of $\mathcal{V}$ without destroying the rigor of the bound and is applicable even when the effect of $\mathcal{V}$ is large. We define, as Bazley does, the projection operator $\mathcal{P}^k$ which projects an arbitrary function $Q\chi$ on to a subspace with k dimensions. The vectors $Q\xi_i$ in this subspace are linearly independent but otherwise arbitrary, with the scalar products defined by $(Q\xi_i,\mathcal{V}Q\xi_j)$. We stress here that, in going from $\mathcal{P}^k$ to $\mathcal{P}^{k+1}$, the old vectors which belong to $\mathcal{P}^k$ space are retained. Then we have

$$\mathcal{P}^kQ\chi=\sum_{i=1}^{k}\alpha_iQ\xi_i\,, \tag{4.8}$$

and the intermediate operators $\mathcal{H}^{(k)}$ are defined by

$$\mathcal{H}^{(k)}=\mathcal{H}_0+\mathcal{V}\mathcal{P}^k\,. \tag{4.9}$$

Obviously, the following inequalities hold:

$$0\leqslant(\mathcal{P}^kQ\chi,\mathcal{U}\mathcal{P}^kQ\chi)\leqslant(Q\chi,\mathcal{U}Q\chi)\,, \tag{4.10}$$

or

$$(Q\chi,\mathcal{K}_0Q\chi)\leqslant(Q\chi,\mathcal{K}^{(k)}Q\chi)\leqslant(Q\chi,\mathcal{K}_vQ\chi)\,, \tag{4.11}$$

which means that

$$\mathcal{E}_i^{(0)}\leqslant\mathcal{E}_i^{(k)}\leqslant\mathcal{E}_i\,,\quad i\leqslant k\,. \tag{4.12}$$

The energies $\mathcal{E}_i$ are for the eigenstates of $\mathcal{K}_v$. So far the procedure has been exactly analogous to that in the bound state problem, but we now have to solve the inhomogeneous equation

$$(\mathcal{K}^{(k)}-E)Q\Psi^{(k)}=-R_0 \tag{4.13}$$

and to evaluate the corresponding bound

$$\Delta^{(k)}=(Q\Psi^{(k)},R_0)=\left(R_0,\frac{1}{Q(E-\mathcal{K}^{(k)})Q}R_0\right). \tag{4.14}$$

From (4.8) we have

$$\mathcal{U}\mathcal{P}^kQ\chi=\sum_{i=1}^{k}\alpha_i\mathcal{U}Q\xi_i\,, \tag{4.15}$$

with

$$\alpha_i=\sum_{j=1}^{k}b_{ij}(Q\xi_j,\mathcal{U}Q\chi)\,. \tag{4.16}$$

b_{ij} are the elements of the inverse of the matrix with $(Q\xi_i,\mathcal{U}Q\xi_j)$. Equation (4.13) becomes, by choosing $Q\xi_i=\mathcal{U}^{-1}Q\Phi_i^{(0)}$,

$$(\mathcal{K}_0-E)Q\Psi^{(k)}+\sum_{i=1}^{k}\sum_{j=1}^{k}b_{ij}(Q\Phi_i^{(0)},Q\Psi^{(k)})Q\Phi_i^{(0)}=-R_0\,. \tag{4.17}$$

Now expand $Q\Psi^{(k)}$ in the form

$$Q\Psi^{(k)}=\sum_{m=1}^{\infty}\alpha_m^{(k)}Q\Phi_m^{(0)}\,, \tag{4.18}$$

which, when substituted into Eq. (4.17), provides the coupled equations for $\alpha_m^{(k)}$, with $m=1,2,\cdots,k$, and the uncoupled equations for all $m>k$:

$$\alpha_m^{(k)}(\mathcal{E}_m^{(0)}-E)+\sum_{n=1}^{k}b_{nm}\alpha_n^{(k)}=-(Q\Phi_m^{(0)},R_0)\,,\quad m\leq k\,, \tag{4.19}$$

$$\alpha_m^{(k)}(\mathcal{E}_m^{(0)}-E)=-(Q\Phi_m^{(0)},R_0)\,,\quad m>k\,. \tag{4.20}$$

Obviously only the first k terms in the expansion (4.18) are affected by the presence of the terms with b_{ij}. Defining the matrix elements of the inverse matrix D^{-1} involved in the solutions of (4.19) by $d_{ij}^{(k)}$, where

$$D_{mn}=(E-\mathcal{E}_m^{(0)})\delta_{mn}-b_{mn}\,, \tag{4.21}$$

with $m,n\leq k$, we have the solutions in the forms

$$\alpha_m^{(k)}=\sum_{n=1}^{k}d_{mn}^{(k)}(Q\Phi_n^{(0)},R_0)\,,\qquad m\leq k\,, \tag{4.22}$$

$$\alpha_m^{(k)}=(E-\mathcal{E}_m^{(0)})^{-1}(Q\Phi_m^{(0)},R_0)\,,\quad m>k\,. \tag{4.23}$$

Substitution of (4.22) and (4.23) into (4.18) gives

$$Q\Psi^{(k)}=\sum_{m,n=1}^{k}d_{mn}(Q\Phi_m^{(0)},R_0)Q\Phi_n^{(0)}+\sum_{m=k+1}^{\infty}\frac{(Q\Phi_m^{(0)},R_0)Q\Phi_m^{(0)}}{E-\mathcal{E}_m^{(0)}}\,. \tag{4.24}$$

$\Delta^{(k)}$ defined by (4.14) now becomes explicitly

$$\Delta^{(k)}=\sum_{m,n=1}^{k}d_{mn}(Q\Phi_m^{(0)},R_0)(Q\Phi_n^{(0)},R_0)+\sum_{m=k+1}^{\infty}\frac{(Q\Phi_m^{(0)},R_0)^2}{E-\mathcal{E}_m^{(0)}}\,. \tag{4.25}$$

Application of the Unsöld approximation and the closure properties of the set $\{Q\Phi_n^{(0)}\}$ to the second sum in (4.25) gives

$$\Delta^{(k)}\geq\Delta_N^{(k)}\,, \tag{4.26}$$

with

$$\Delta_N^{(k)}=\sum_{m,n=1}^{k}d_{mn}(Q\Phi_m^{(0)},R_0)(Q\Phi_n^{(0)},R_0)+(R_0,R_0)/(E-\mathcal{E}_{N+1}^{(0)})+\sum_{m=k+1}^{N}\frac{(Q\Phi_m^{(0)},R_0)^2}{E-\mathcal{E}_m^{(0)}}-\sum_{m=1}^{N}\frac{(Q\Phi_m^{(0)},R_0)^2}{E-\mathcal{E}_{N+1}^{(0)}}\,, \tag{4.27}$$

where $N\geq k+1$. This is the desired result which reduces to (4.7) for the case $k=0$. It does not contain the $\mathcal{K}^2$ operator as in the previous section and the resulting bound is a rigorous one on the assumption that the effect of $\mathcal{U}$ can be neglected.

Before discussing the method to include $\mathcal{U}$, we investigate a little further to see if one can do better than (4.27). $\Delta_N^{(k)}$ involves $\mathcal{E}_n^{(0)}$ in all the sums except in the first term, and the appearence of $\mathcal{E}_{N+1}^{(0)}$ is undesirable since, if the effect of $\mathcal{U}$ is large, it may be a very bad bound on $\mathcal{E}_{N+1}$ and it may sometimes be possible that $\mathcal{E}_k^{(k)}$ lies above $\mathcal{E}_{N+1}^{(0)}$. In fact, it is *not* necessary to restrict the problem from the beginning as in (4.13), but rather consider instead the quantity

$$\Delta_v=(R_0,G^QR_0)=\sum_{n=1}^{\infty}(R_0,Q\Phi_n)^2/(E-\mathcal{E}_n) \tag{4.28}$$

$$=\sum_{n=1}^{k}\frac{(R_0,Q\Phi_n)^2}{E-\mathcal{E}_n}+\sum_{n=k+1}^{\infty}\frac{(R_0,Q\Phi_n)^2}{E-\mathcal{E}_n}\,. \tag{4.29}$$

Replacing the first sum in terms of the result (4.22), and applying the Unsöld approximation and completeness to the second sum, we have

$$\Delta_v \geqslant \sum_{m,n=1}^{k} d_{mn}(Q\Phi_m{}^{(0)},R_0)(Q\Phi_n{}^{(0)},R_0) + \frac{(R_0,R_0)}{E-\mathcal{E}_{k+1}} - \sum_{m=1}^{k} \frac{(R_0,Q\Phi_m)^2}{E-\mathcal{E}_{k+1}}. \quad (4.30)$$

The bound given by (4.30) is presumably superior to (4.27), only if the last term can be evaluated. (This last term gives a positive contribution and thus can be neglected entirely, but one can improve the bound by properly evaluating this term.) For this purpose we rewrite (4.29) in the form

$$\Delta_v \geqslant \frac{(R_0,R_0)}{E-\mathcal{E}_{k+1}} + \sum_{n=1}^{k} \frac{(R_0,Q\Phi_n)^2}{E-\mathcal{E}_n} \cdot \frac{(\mathcal{E}_n-\mathcal{E}_{k+1})}{(E-\mathcal{E}_{k+1})}.$$

From this it follows that, using the result of (4.22),

$$\Delta_v \geqslant \frac{(R_0,R_0)}{E-\bar{E}_{k+1}} + \sum_{m,n=1}^{k} d_{mn}(Q\Phi_m{}^{(0)},R_0) \times (Q\Phi_n{}^{(0)},R_0) \frac{\bar{E}_n-\bar{E}_{k+1}}{E-\bar{E}_{k+1}} = \frac{(R_0,R_0)}{E-\bar{E}_{k+1}} + \sum_{n=1}^{k} \frac{(R_0,Q\bar{\Phi}_n)^2}{E-\bar{E}_n} \cdot \frac{(\bar{E}_n-\bar{E}_{k+1})}{(E-\bar{E}_{k+1})}. \quad (4.31)$$

In (4.31), the energy values $\bar{E}_n$ and the wave functions $Q\bar{\Phi}_n$ have been obtained by diagonalizing the D matrix defined by (4.21).

The lower bound (4.31) has been derived with the assumption that $\mathcal{E}_n > E$ for all n. In case there are $N_v{}^Q$ negative eigenvalues of the operator $Q(\mathcal{H}_v-E)Q$, then the form of (4.31) should be slightly modified to the form

$$\Delta_v \geqslant \frac{(R_0,R_0)}{E-\bar{E}_{k+1}} + \sum_{n=1}^{N_v{}^Q} \frac{(R_0,Q\bar{\Phi}_n)^2}{E-\bar{E}_n} \cdot \frac{(\bar{E}_n-\bar{E}_{k+1})}{(E-\bar{E}_{k+1})} + \sum_{n=N_v{}^Q+1}^{k} \frac{(R_0,Q\bar{\Phi}_n)^2}{E-\bar{E}_n} \cdot \frac{(\bar{E}_n-\bar{E}_{k+1})}{(E-\bar{E}_{k+1})}, \quad (4.32)$$

where $\bar{E}_n$ are the lower bounds obtained by the diagonalization of D as before and $\bar{E}_n$ are the upper bounds which can always be obtained by the variational method of Ritz.

C. Energy Shift Operator

When the effect of $\mathfrak{U}$ on Δ is small, we can treat $\mathfrak{U}$ by perturbation theory. As will be discussed in the next section, however, the "smallness" of $\mathfrak{U}$ in the operator $\mathcal{H}$ does not necessarily imply that its effect is also small in Δ. Thus, although $\mathfrak{U}$ is small compared to $\mathcal{V}$, the series

$$\bar{G}^Q = \sum_{n=0}^{\infty} (G^Q\mathfrak{U})^n \cdot G^Q \quad (4.33)$$

may not converge. If the series converges rapidly, then a sensible estimate of the effect of $\mathfrak{U}$ can be obtained either by taking one or two terms in the perturbation series or by the modification of the Green's function G^Q by

$$G^Q \equiv [Q(E-\mathcal{H}_v)Q]^{-1} \rightarrow [Q(E-\langle\mathfrak{U}\rangle-\mathcal{H}_v)Q]^{-1}, \quad (4.34)$$

where

$$\langle\mathfrak{U}\rangle \equiv (Q\Psi_t,\mathfrak{U}Q\Psi_t).$$

The advantage of (4.34) is that by replacing E by $\bar{E} \equiv E-\langle\mathfrak{U}\rangle$, the entire formulation of part B can be immediately applied without further change.

It is also possible to treat the problem by the iteration method of Appendix A. From Eqs. (2.3) and (2.4), it is reasonable to expect that, instead of modifying the Green's function G^Q directly, we can also modify R_0 by replacing $P\Psi^P$ by an appropriately defined function $P\bar{\Psi}$. Therefore, to correct the result (4.32) we need the explicit expression for $Q\Psi_k$ which should be inserted into the right hand side of Eq. (2.3). Comparison of (4.32) with Δ and Δ_k, given by

$$\Delta = (Q\Psi,R_0), \quad (4.35)$$

$$\Delta_k = (Q\Psi_k,R_0), \quad (4.36)$$

suggests that we may write

$$Q\Psi_k = \frac{R_0}{E-\bar{E}_{k+1}} + \sum_{n=1}^{N_v{}^Q} \frac{(R_0,Q\bar{\Phi}_n)}{E-\bar{E}_n} \cdot \frac{(\bar{E}_n-\bar{E}_{k+1})}{(E-\bar{E}_{k+1})} Q\bar{\Phi}_n + \sum_{n=N_v{}^Q+1}^{k} \frac{(R_0,Q\bar{\Phi}_n)}{E-\bar{E}_n} \cdot \frac{(\bar{E}_n-\bar{E}_{k+1})}{(E-\bar{E}_{k+1})} Q\bar{\Phi}_n. \quad (4.37)$$

The function $Q\Psi_k$ of (4.37) is a pseudofunction which should only be used in the expression for Δ. Substituting $Q\Psi_k$ into the P equation,

$$P(H-E)P\Psi_k = -PHQ\Psi_k, \quad (4.38)$$

and solving for $P\Psi_k$ *exactly*, we obtain the modified $R_k = QHP\Psi_k$. This, in turn, can be substituted into (4.37) in place of R_0, and the new $Q\Psi_k$ is derived. Repetition of this iteration cycle until it converges gives

$$\Delta_L = (Q\Psi_k,R_0). \quad (4.39)$$

The step involved in (4.38) can also be seen in terms of the Green's function $G_k{}^Q$ defined by

$$G_k{}^Q = \frac{Q}{E-\bar{E}_{k+1}} + \sum_{n=1}^{N_v{}^Q} \frac{Q\bar{\Phi}_n)(Q\bar{\Phi}_n}{E-\bar{E}_n} \cdot \frac{\bar{E}_n-\bar{E}_{k+1}}{E-\bar{E}_{k+1}} + \sum_{n=N_v{}^Q+1}^{k} \frac{(Q\bar{\Phi}_n)(Q\bar{\Phi}_n)}{E-\bar{E}_n} \cdot \frac{\bar{E}_n-\bar{E}_{k+1}}{E-\bar{E}_{k+1}}. \quad (4.40)$$

The solution $P\Psi_k$ of the equation

$$P(H+HG_k{}^QH-E)P\Psi_k=0, \tag{4.41}$$

gives the bound

$$\Delta\geqslant\Delta_L=(P\Psi^P,HG_k{}^QHP\Psi_k), \tag{4.42}$$

which is completely equivalent to (4.39). The lower bound given by (4.39) and (4.42) is *rigorous* only if the iteration process described above converges. For a reasonably accurate $Q\Psi_k$ and for E not too close to one of the eigenvalues of $\mathcal{H}$, we expect that the convergence would be rapid.

D. Different Choices

(i) In part B, we have chosen the particular splitting of the original $\mathcal{H}$ in the form $\mathcal{H}=\mathcal{H}_0+\mathcal{V}+\mathcal{U}$, with $\mathcal{V}>0$. We neglect again the interaction $\mathcal{U}$ in the following discussion. For $\mathcal{V}>0$, what we have actually done is to replace the operator $\mathcal{V}$ by a lower bound $\mathcal{V}^{(k)}$ defined by

$$\mathcal{V}\geqslant\mathcal{V}^{(k)}\equiv\mathcal{V}|\xi)\mathbf{D}^{-1}(\xi|\mathcal{V}\geqslant 0, \tag{4.43}$$

where $\mathbf{D}$ is the matrix with

$$D_{ij}=(\xi_i,\mathcal{V}\xi_j) \tag{4.44}$$

and we will use the vector notation throughout. The inequality (4.43) can be proved by minimizing the quantity $(\chi,\mathcal{V}\chi)$ with respect to the parameters c_i contained in an arbitrary real function $\chi=\chi_0+\sum_{i=1}^{k}c_i\xi_i$. Next, particular forms for ξ_i are chosen so that the resulting coupled set of equations can be solved exactly for $Q\Psi^{(k)}$; we choose

$$\xi_i=\mathcal{V}^{-1}Q\Phi_i{}^{(0)}, \quad i=1,2,\cdots,k, \tag{4.45}$$

where $Q\Phi_i{}^{(0)}$ are the eigenfunctions of $\mathcal{H}_0$. We then have

$$\mathcal{H}_0\leqslant\mathcal{H}^{(k)}\leqslant\mathcal{H}_v \tag{4.46}$$

with

$$\mathcal{H}^{(k)}=\mathcal{H}_0+\mathcal{V}^{(k)}. \tag{4.47}$$

(4.46) in turn gives, with $G_k{}^Q=Q(E-\mathcal{H}^{(k)})Q$,

$$Q(E-\mathcal{H}_0)Q^{-1}=G_0{}^Q\leqslant G_k{}^Q\leqslant G^Q=Q(E-\mathcal{H}_v)Q^{-1} \tag{4.48}$$

and finally we have

$$\Delta_0\leqslant\Delta^{(k)}\leqslant\Delta_v. \tag{4.49}$$

Assuming that $G_0{}^Q$ cannot be evaluated exactly, we have expounded in part B a method to bound $\Delta^{(k)}$ in manageable forms for practical application.

(ii) It is also possible to split $\mathcal{H}_v-EQ$ in a different form, as Blankenbecler and Sugar do.[10] We write in a slightly generalized form

$$\mathcal{H}_v-E=(\mathcal{H}_v-\tilde{\epsilon})-(E-\tilde{\epsilon}), \tag{4.50}$$

where $\tilde{\epsilon}$ is chosen as in Sec. III

$$E<\tilde{\epsilon}\leqslant\mathcal{E}_1. \tag{4.51}$$

Then we have the analog of (4.43),

$$F\geqslant F_s=F|\xi)\mathbf{M}^{-1}(\xi|F\geqslant 0, \tag{4.52}$$

where

$$F\equiv(\mathcal{H}_v-\tilde{\epsilon})/(\tilde{\epsilon}-E)>0, \tag{4.53}$$

$$\mathbf{M}=(\xi|F|\xi). \tag{4.54}$$

Using (4.52), we have

$$G^Q=(E-\tilde{\epsilon})^{-1}(1+F)^{-1}\geqslant(E-\tilde{\epsilon})^{-1}(1+F_s)^{-1} \tag{4.55}$$

and

$$\Delta_v\geqslant\frac{1}{E-\tilde{\epsilon}}\left[(R_0,R_0)-\frac{(R_0,F\xi)^2}{(\xi,F\xi)(\xi,F^2\xi)}\right]. \tag{4.56}$$

The advantage of the choice (4.50) is that the factor $(1+F_s)^{-1}$ in (4.55) *can be readily inverted* without the application of the Unsöld approximation and without invoking the closure property, due to the fact that F_s is essentially separable. Unfortunately, (4.56) involves again the operator $\mathcal{H}$ in quadratic form, and therefore should be compared with (3.11). They are similar but not equivalent.

(iii) There is still another choice, among probably many more, which has to do with the choice of the vector ξ; instead of (4.45), we can try the form, following Gay,[11]

$$\xi=\mathcal{V}^{-1}(\mathcal{H}_0-EQ)|\mathbf{f}), \tag{4.57}$$

where the new vector $\mathbf{f}$ may not have anything to do with the eigenfunctions $Q\Phi^{(0)}$ of $\mathcal{H}_0$. With this choice, we have

$$\begin{aligned}\mathbf{D}&=(\xi,\mathcal{V}\xi)\\&=(\mathbf{f}|(\mathcal{H}_0-EQ)\mathcal{V}^{-1}(\mathcal{H}_0-EQ)|\mathbf{f}).\end{aligned} \tag{4.58}$$

The lower bound on the potential $\mathcal{V}$ is

$$\begin{aligned}\mathcal{V}&\geqslant\mathcal{V}|\xi)\mathbf{D}^{-1}(\xi|\mathcal{V}\\&=(\mathcal{H}_0-EQ)|\mathbf{f})\mathbf{D}^{-1}(\mathbf{f}|(\mathcal{H}_0-EQ)\geqslant 0,\end{aligned}$$

and the Green's function G^Q is bounded by

$$\begin{aligned}G^Q&\geqslant[1-|\mathbf{f})\mathbf{D}^{-1}(\mathbf{f}|(\mathcal{H}_0-EQ)]^{-1}[Q(E-\mathcal{H}_0)Q]^{-1}\\&=[1+|\mathbf{f})\{(\mathbf{f}|(\mathcal{H}_0-E)\mathcal{V}^{-1}(\mathcal{H}_0-E)|\mathbf{f})\\&-(\mathbf{f}|(\mathcal{H}_0-E)|\mathbf{f})\}^{-1}(\mathbf{f}|(\mathcal{H}_0-E)][Q(E-\mathcal{H}_0)Q]^{-1}.\end{aligned} \tag{4.59}$$

The part of (4.59) in the square bracket can be evaluated exactly as in (4.56), while the Green's function $G_0{}^Q$ still needs an approximation such as the one performed in part A. Thus, the choice (4.57) is intermediate between the choices (4.45) and (4.50).

[10] R. Sugar and R. Blankenbecler, Phys. Rev. **136**, B472 (1964). We add the remark here that their formulation of the upper bound on Δ is equivalent to the formulation of Ref. 3, as can be seen by the relation $Q\Psi=G^QQHP\Psi=\bar{G}^QQHP\Psi^P$. They emphasize on the other hand the construction of a variational approximation for G^Q and then require the exact solution of the P equation with G^Q replaced by $G_t{}^Q$, while in Ref. 3 a variational approximation to Δ directly in terms of $Q\Psi_t$ is stressed.

[11] J. G. Gay, Phys. Rev. **135**, A1220 (1964).

V. CONVERGENCE OF ITERATION SERIES

In Sec. IV the iteration method was formulated to take into account the effect of the shift operator $\mathfrak{U}$. A similar method is given in Appendix A which avoids the explicit evaluation of G^P appearing in $\mathfrak{IC}$. These methods presuppose the rapid convergence of the iteration series, and in this section we discuss the necessary and sufficient conditions under which the series is guaranteed to converge. Of course, in the variation-iteration method of Appendix A, for example, the Green's function G^Q is not known exactly but only approximately in a variational sense. However, for clarity of discussion, we assume that G^Q is known exactly. The complication due to the fact that we are using an approximate G^Q can be easily taken into account afterward.

The convergence of the series can be treated in a general way in terms of the problem involving two potentials $\mathfrak{U}$ and $\mathfrak{V}$. Define the Green's functions for the various operators connected with $\mathfrak{IC}$, where

$$\begin{aligned}\mathfrak{IC}&=\mathfrak{IC}_0+\mathfrak{V}+\mathfrak{U}\\&=\mathfrak{IC}_v+\mathfrak{U}, \quad (\mathfrak{IC}_v\equiv QHQ),\end{aligned} \tag{5.1}$$

by

$$\begin{aligned}(\mathfrak{IC}_0-E)QG_0{}^Q&=-Q\delta,\\(\mathfrak{IC}_v-E)QG^Q&=-Q\delta,\\(\mathfrak{IC}-E)Q\bar{G}^Q&=-Q\delta,\end{aligned} \tag{5.2}$$

where we take the principal value integrals for the Green's functions. The relevant transition operators in Q space for the present problem are

$$T_v=\mathfrak{V}+\mathfrak{V}G_0{}^QT_v \tag{5.3}$$

and

$$\begin{aligned}T&=\mathfrak{U}+\mathfrak{U}G^QT\\&=\mathfrak{U}+\mathfrak{U}\bar{G}^Q\mathfrak{U}.\end{aligned} \tag{5.4}$$

(5.4) can also be expressed in terms of T_v as

$$T=T_v+(1+T_vG_0{}^Q)\mathfrak{U}(G_0{}^QT+1). \tag{5.5}$$

The quantity of interest Δ as defined by (3.10) can be written in the form

$$\begin{aligned}\Delta&=(R_0,\bar{G}^QR_0)\\&=(R_0,[G_0{}^Q+G_0{}^QTG_0{}^Q]R_0),\end{aligned} \tag{5.6}$$

where the relation

$$\begin{aligned}\bar{G}^Q&=G_0{}^Q+G_0{}^Q(\mathfrak{V}+\mathfrak{U})\bar{G}^Q\\&=G_0{}^Q+G_0{}^QTG_0{}^Q\end{aligned} \tag{5.7}$$

is used. A more convenient form than (5.5) for T is obtained by solving the integral Eq. (5.5) for T formally and is given by

$$\begin{aligned}T&=(T_v+\mathfrak{W})+\mathfrak{W}\mathcal{G}^Q(T_v+\mathfrak{W})\\&=\mathcal{T}+\mathcal{T}\mathcal{G}^Q\mathfrak{W},\end{aligned} \tag{5.8}$$

where

$$\mathfrak{W}\equiv\mathfrak{U}+T_vG_0{}^Q\mathfrak{U}, \tag{5.9}$$

$$\mathcal{G}^Q\equiv[Q(E-\mathfrak{IC}_0-\mathfrak{W})Q]^{-1}, \tag{5.10}$$

$$\mathcal{T}\equiv\mathfrak{W}+T_v. \tag{5.11}$$

From (5.8) it is reasonable to expect that if the number of poles contained in T differs from that of T_v, then $\mathcal{G}^Q$ should have zeros and poles in order to compensate for the difference. In such cases, the expansion of $\mathcal{G}^Q$ in a series involving either $G_0{}^Q$ or G^Q is not expected to converge. The convergence problem of the series

$$\mathcal{G}^Q=\sum_{n=0}^{\infty}(G_0{}^Q\mathfrak{W})^nG_0{}^Q \tag{5.12}$$

is equivalent to the question for the series

$$\bar{G}^Q=\sum_{n=0}^{\infty}(G^Q\mathfrak{U})^nG^Q \tag{5.13}$$

because of the identity $G_0{}^Q\mathfrak{W}=G^Q\mathfrak{U}$. (5.13) is what is also involved in the iteration methods of Sec. IV and Appendix A.

To make our argument a little more precise, we now consider the potential strength eigenvalue problem for the kernel $G^Q\mathfrak{U}$, which was found to be very convenient for discussion of the convergence question.[12] We have

$$G^Q\mathfrak{U}|\gamma_n\rangle=\gamma_n|\gamma_n\rangle, \tag{5.14}$$

or, what is the same thing,

$$Q(H+(\mathfrak{U}/\gamma_n)-E)Q|\gamma_n\rangle=0.$$

The series (5.13) can be expressed for the state $|\gamma_n\rangle$ as

$$\bar{G}^Q\mathfrak{U}|\gamma_n\rangle=\sum_{m=0}\gamma_n{}^{m+1}|\gamma_n\rangle. \tag{5.15}$$

Obviously, the series (5.15) diverges if, for any n,

$$|\gamma_n|\geq 1, \tag{5.16}$$

while it can be summed to be $(1-\gamma_n)^{-1}\gamma_n|\gamma_n\rangle$ if $|\gamma_n|<1$ for all n. It is well known that for each γ_n which leaves the unit circle the operator $Q(\mathfrak{IC}-E)Q$ associated with T either gains or loses one negative energy state of the operator $Q(\mathfrak{IC}_v-E)Q$ associated with T_v. Therefore, in general, if the operator $Q(\mathfrak{IC}-E)Q$ has N^Q negative eigenvalues while the operator $Q(\mathfrak{IC}_v-E)Q$ has $N_v{}^Q$, there will be $|N^Q-N_v{}^Q|$ γ's which leave the unit circle, i.e., $|\gamma_n|\geq 1$ for $n=1, 2, \cdots, |N^Q-N_v{}^Q|$. Thus, when the operator $\mathfrak{U}$ is such that the nth state of $\mathfrak{IC}$ and $\mathfrak{IC}_v$, with the eigenvalues $\mathcal{E}_n{}^Q$ and $\mathcal{E}_n$, respectively, satisfies

$$\mathcal{E}_n{}^Q\gtrless\mathcal{E}_n, \tag{5.17}$$

then it follows immediately that the iteration series (5.13) or (5.15) diverges if and only if E lies between the two values

$$\mathcal{E}_n{}^Q\gtrless E\gtrless\mathcal{E}_n. \tag{5.18}$$

[12] S. Weinberg, Phys. Rev. **131**, 440 (1963); **133**, B232 (1964).

In fact, the series diverges even if $\mathfrak{U}$ is very weak, as soon as E satisfies (5.18). This is peculiar to the multipotential problem and is due to the fact that the expression for Δ, (5.6), involves $\bar{G}^Q$. Thus a small perturbation of the operator $\mathfrak{K}$ in the denominator may cause a violent behavior in Δ if E happens to be very close to one of the eigenvalues of $\mathfrak{K}$. A similar divergence problem is often encountered when one tries to evaluate the scattering parameters near a sharp resonance by a perturbation method.

The above discussion immediately suggests the remedy in case the series either diverges or is very slowly converging. It is only necessary to add an arbitrary potential $\mathfrak{Y}$ to $\mathfrak{K}_v$ such that the eigenstates corresponding to the new operator $\mathfrak{K}_v' \equiv \mathfrak{K}_v + \mathfrak{Y}$ satisfy the inequalities

$$E \gtrless \mathcal{E}_n{}^Q,\ \mathcal{E}_n'. \tag{5.19}$$

The effect of the operator can be corrected by the modified inhomogeneous term and can be treated as part of the iteration. With $\mathfrak{U}' = \mathfrak{U} - \mathfrak{Y}$, the modified iteration series involves $G^{Q'}\mathfrak{U}'$ instead of $G^Q\mathfrak{U}$, and the series converges since now $N^Q = N_{v'}{}^Q$. For the method described in Sec. IV, the addition of $\mathfrak{Y}$ may complicate the problem, and it seems that the simplest way may be to vary the strength of the potential $\mathfrak{V}$ by adjusting the over-all strength constant.

So far the discussion has been given under the assumption that the Green's function G^Q is known exactly. In an actual application this is not usually the case, unless the Q space is truncated for convenience, as in the close-coupling approximation. If G^Q is assumed known approximately from a minimum principle calculation, for example, then we have

$$\mathcal{E}_{nt}{}^Q \geq \mathcal{E}_n{}^Q. \tag{5.20}$$

We conclude from (5.18) and (5.20) that the modification of the form (5.19) with $\mathfrak{Y} < 0$ is definitely required in order to have the series convergent if $\langle \mathfrak{U} \rangle < 0$, while, if $\langle \mathfrak{U} \rangle > 0$, then the approximate Green's function $G_t{}^Q$ will help the convergence as long as $\mathcal{E}_{nt} > E$

VI. DISCUSSION

The expressions for the upper bound given by (2.12) or (2.14) and the lower bounds given by (3.16) and (3.21) in quadratic forms and (4.39) in linear form are all exact, while many other approximate bounds are also given during the various intermediate steps. Even with the exact bounds, it is almost always necessary for computational reasons to relax the rigor and substitute various approximate quantities in the formulas in order to apply them in a practical calculation. Moreover, none of the lower bounds obtained thus far are of the truly variational character with the linear operator $\mathfrak{K}$. This shortcoming is inherent in the problem with the operator $\mathfrak{K}$ having the spectral properties discussed earlier, and it does not seem possible to derive a maximum principle as general as the minimum principle (2.12).

Due to the discreteness of the spectrum of $\mathfrak{K}$, on the other hand, a rigorous discussion of the convergence properties of the iteration series can be given; the kernel $G^Q\mathfrak{U}$ is square integrable for a reasonably well behaved potential $\mathfrak{U}$, and it is not necessary to introduce the complex energy E nor complex γ_n, as would be the case if one were to deal with the original Hamiltonian H directly.[12] It is also trivial to note that the question of the connectedness of the Green's function and the kernel in the case of many-particle scattering does not arise with the operator $\mathfrak{K}$, simply because in the present formalism, as in Feshbach's formulation of the reaction theory, we presuppose that the target system with N particles is completely known in terms of P and Q operators. Only the interaction between the incoming particle and the target is in question. The interaction potential V is the sum of two-particle interactions, but it is smoothed out by the operation PVQ and thus completely connected.

For the choice of the constant vector **a** in (2.13), the detailed discussion has been given in Ref. 3. By different choices we obtain bounds on the diagonal elements of the inverse reactance matrix, or on the appropriate linear combinations of the matrix elements. Since we now have the methods to calculate lower bounds as well as the upper bounds, it is trivial to show that similar bounds can be obtained on any individual elements of the inverse reactance matrix.

It is not likely that the requirement on P and $P\Psi^P$ can be easily relaxed. However, from the fact that the usual Kohn variational principle often gives an upper bound when a large number of parameters are put into the trial function, it is very plausible, although the proof cannot be given, that the requirement of the strong operator identity (A2) may be replaced by a weaker identity of the form

$$(P\Psi_t, [H-E]P\Psi_t) = -(P\Psi_t, PHQ\Psi_t).$$

If this were true, then we could write down a more general minimum principle of the form

$$\lambda_M = \lambda_t + (\Lambda P\Psi_t + Q\Psi_t, [H-E]\Psi_t),$$

where Λ is a Lagrangian multiplier. We note that, as expected, λ_M reduces for $\Lambda = 1$ to Kohn's variational principle.

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APPENDIX A: VARIATION-ITERATION METHOD

The Green's function G^P appears in Eq. (2.11) when the two coupled Eqs. (2.3) and (2.4) are uncoupled

using the solutions (2.5) and (2.6). Therefore, in order to eliminate G^P from the operator $\mathcal{H}$, we may have to go back to the original coupled equations and try to solve them directly by iterations. The P equation (2.3) is rather easy to solve once the inhomogeneous term is given, while the Q equation (2.4) can only be solved either variationally or perhaps by perturbation methods.

The variation-iteration method to be described here specifically avoids the explicit evaluation of G^P, and is essentially based on the simple observation that it is not any more difficult to solve the inhomogeneous Eq. (2.3) than the homogeneous one (2.7), which is required in order to have a bound on λ. A similar technique has been frequently used in the past, especially in evaluating various sum rules involved in atomic problems.[13] The method consists of the following three steps:

(a) Construction of the trial function $Q\Psi_t$ which satisfies the boundary conditions but is otherwise arbitrary. $Q\Psi_t=0$ is one simple choice. Or, the Q equation may be solved *variationally* using a reasonable function $P\Psi_t$, for example $P\Psi^P$. Thus we have

$$\delta[(Q\Psi_t,[H-E]Q\Psi_t)+2(Q\Psi_t,QHP\Psi_t)]=0. \quad \text{(A1)}$$

(b) $Q\Psi_t$ thus obtained is substituted into the r.h.s. of the P equation and the resulting equation is solved *exactly* for $P\tilde{\Psi}_t$:

$$P(H-E)P\tilde{\Psi}_t=-PHQ\Psi_t. \quad \text{(A2)}$$

(c) For the pair of functions $Q\Psi_t$ and $P\tilde{\Psi}_t$ obtained by the steps (a) and (b), we can show from the minimum principle (2.12) that

$$\lambda\leqslant\lambda^M, \quad \text{(A3)}$$

where

$$\lambda^M=\lambda_t+(Q\Psi_t,[H-E][Q\Psi_t+P\tilde{\Psi}_t]). \quad \text{(A4)}$$

In deriving (A4), the following identities are used:

$$P\tilde{\Psi}_t=P\Psi^P+G^PHQ\Psi_t \quad \text{(A5)}$$

$$\lambda_t=\lambda^P+(P\Psi^P,PHQ\Psi_t). \quad \text{(A6)}$$

We have neglected the possibility of the presence of subtraction terms. It is connected with the problem of resonance states and also with the convergence problem of the iteration series, and has been discussed in Sec. V.

The method can be demonstrated for the simple choice $Q\Psi_{0t}=0$. This corresponds directly to the usual procedure adapted in the close-coupling approximation, in which the Q equations are truncated to a finite number of coupled equations and the reduced set of P and Q equations are solved exactly numerically.

*0*th *iteration:*

(a) $Q\Psi_{0t}=0$.

(b) $P\tilde{\Psi}_{0t}$ is obtained by solving the P equation exactly,

$$P(H-E)P\tilde{\Psi}_{0t}=-PHE\Psi_{0t}=0.$$

The solution is the usual static approximation.

(c) From (a) and (b), we have

$$\lambda\leqslant\lambda_0{}^M=\lambda^P.$$

*1*st *iteration:*

(a) $P\tilde{\Psi}_{0t}$ is substituted in the r.h.s. of the Q-equation and we solve for $Q\Psi_{1t}$ *variationally*,

$$\delta[(Q\Psi_{1t},[H-E]Q\Psi_{1t})+2(Q\Psi_{1t},QHP\tilde{\Psi}_{0t})]=0.$$

(b) $Q\Psi_{1t}$ is substituted into the r.h.s. of the P equation and we solve for $P\tilde{\Psi}_{1t}$ *exactly*,

$$P(H-E)P\tilde{\Psi}_{1t}=-PHQ\Psi_{1t}.$$

(c) Then, from (a) and (b) above, we have

$$\lambda\leqslant\lambda_1{}^M=\lambda^P+(Q\Psi_{1t},QHP[P\Psi^P+P\tilde{\Psi}_{1t}-P\tilde{\Psi}_{0t}]).$$

After the nth iteration, we have

$$\begin{aligned}\lambda\leqslant\lambda_n{}^M&=\lambda_{nt}+(Q\Psi_{nt},QHP[P\tilde{\Psi}_{nt}-P\tilde{\Psi}_{n-1,t}])\\&=\lambda_{n-1,t}+(Q\Psi_{nt}-Q\Psi_{n-1,t},QHP\tilde{\Psi}_{nt}). \quad \text{(A7)}\end{aligned}$$

The λ_{nt} which is introduced in (A7) can be read off from the asymptotic form of $P\tilde{\Psi}_{nt}$. Assuming that the iteration series converges rapidly, (A7) provides thus a *rigorous upper bound on* λ *at every stage* of the iteration.

In the close-coupling approximation, as mentioned earlier, a finite number of exact states are selected from Q states, and then resulting coupled set of equations are solved exactly. The variational principle, on the other hand, treats the entire Ψ approximately. Therefore, the variation-iteration method given here is a suitable combination of the two methods in such a way that the resulting λ^M gives a rigorous bound.

Finally, it is a simple matter to convert the result of the usual variational calculation and obtain a rigorous bound. From the variational principle we have

$$\lambda^V=\lambda_t+(\Psi_t,[H-E]\Psi_t).$$

Following the steps (a), (b), and (c), we obtain

$$\begin{aligned}\lambda&\leqslant\lambda_M{}^V\\&=\tilde{\lambda}_t+(Q\Psi_t,[H-E]\tilde{\Psi}_t), \quad \text{(A8)}\end{aligned}$$

where

$$\tilde{\Psi}_t\equiv P\tilde{\Psi}_t+Q\Psi_t$$

$\tilde{\lambda}_t=\lambda_t$ associated with the function $P\tilde{\Psi}_t$.

APPENDIX B: FLUCTUATION POTENTIALS

In the usual phenomenological analysis of scattering problems in atomic and nuclear theories, one often assumes an optical potential of arbitrary form with certain prescribed behaviors at the origin and at infinity in coordinate space. On the other hand the fluctuation potential given by (3.14) has a definite physical

[13] R. M. Sternheimer, Phys. Rev. **96**, 951 (1954); A Dalgarno and A. Stewart, Proc. Roy. Soc. (London) **A238**, 269 and 276 (1956); C. Schwartz, Ann. Phys. (N. Y.) **6**, 170 (1959).

interpretation and can be evaluated without the detailed knowledge of $Q\Psi$. Therefore it is of some interest to study the explicit behavior in simple cases in which the total Hamiltonian H is given.

In the case of single-channel elastic scattering of positrons by atomic hydrogen, we have $P=|\psi_{T0})(\psi_{T0}|$ with $\psi_{T0}=2\exp(-r_1)$ and $V=2(r_2^{-1}-r_{12}^{-1})$, where r_1 and r_2 are the distances from the fixed proton of the electron and the positron, respectively, and we have used the atomic units for energies and the Bohr radius for the unit of lengths. The explicit form of the fluctuation potential $\langle V\rangle$ can be obtained for this case; dropping the projection operator P which is present by definition, we have

$$(E-\tilde{\epsilon})\langle V\rangle=-(4/r_2^2)(1-e^{-2r_2})^2+(8/r_2)(1-e^{-2r_2})e^{-2r_2}-4e^{-4r_2}-4\Big[(e^{2r_2}+e^{-2r_2})\int_{r_2}^{\infty}\frac{e^{-2y}}{y}dy$$
$$-e^{-2r_2}\int_0^{r_2}\frac{(e^{2y}-e^{-2y})}{y}dy\Big]+\frac{2}{r_2}\Big[(e^{2r_2}-e^{-2r_2})\int_{r_2}^{\infty}\frac{e^{-2y}}{y}dy+e^{-2r_2}\int_0^{r_2}\frac{(e^{2y}-e^{-2y})}{y}dy\Big].$$

The constant $\tilde{\epsilon}$ is so far arbitrary and can be chosen to simulate the true potential when this is possible. It behaves as

$$\langle V\rangle\sim(E-\tilde{\epsilon})^{-1}(4+\mathcal{O}(r_2^2,r_2^2\ln 2r_2,\cdots)),\quad r_2\approx 0$$
$$\langle V\rangle\to(E-\tilde{\epsilon})^{-1}(4r_2^{-4}+\mathcal{O}(r_2^{-6})),\quad r_2\to\infty.$$

When $\tilde{\epsilon}$ is chosen to be $\tilde{\epsilon}=-\frac{1}{9}$,[14] and the total energy E is $E=-1$ corresponding to the zero energy scattering, $\langle V\rangle$ behaves asymptotically as

$$\langle V\rangle\to-(\tfrac{9}{2})r_2^{-4}$$

as expected. On the other hand, we can use the most likely lower bound $\tilde{\epsilon}=-\frac{1}{2}$, which corresponds to the threshold energy for the pickup process, and obtain the asymptotic behavior $-8r_2^{-4}$.

A similar calculation can also be carried out for the elastic scattering of electrons by atomic hydrogen. In this case, $\langle V\rangle$ becomes more involved due to the exchange effect. However, its asymptotic behavior is exactly the same as in the e^+H case, since the exchange effect is of short range. We give here the explicit form of the P equation with the fluctuation potential:

$$\Big[T_1+V_1+V_{00}-E+E_{T0}+\frac{1}{E-\tilde{\epsilon}}\{(V^2)_{00}-(V_{00})^2\}\Big]\bar{u}_0(r_1)$$
$$\pm\psi_{T0}(r_1)\Big[\int dr_2'\psi_{T0}(r_2')\Big\{V+2E_{T0}-E+\frac{V^2-V_{00}(r_1)V}{E-\tilde{\epsilon}}\Big\}\bar{u}_0(r_2')$$
$$-\frac{1}{E-\tilde{\epsilon}}\int dr_2'\psi_{T0}(r_2')V\{\bar{u}_0(r_2')V_{00}(r_2')\pm\psi_{T0}(r_2')dr_1'\psi_{T0}(r_1')V\bar{u}_0(r_1')\}\Big]=0.$$

We used the notations: T_1 is the kinetic operator for the particle 1, $V_1=-2/r_1$, $V_{00}=-2(1+r_1^{-1})\exp(-2r_1)$, $\pm$ signs are positive for the singlet and negative for the triplet states. In the present case, the rigorous lower bound $\tilde{\epsilon}$ is also known,[6] which gives the asymptotic behavior roughly of the form $\langle V\rangle\to-(16/3)r_1^{-4}$.

APPENDIX C: VARIATIONAL PRINCIPLES FOR THE STRENGTH EIGENVALUES

A variational principle for the calculation of the strength eigenvalues ζ_n associated with the interaction operator $\mathcal{H}^{(1)}=\mathcal{H}-\mathcal{H}^{(0)}$ will now be described. Variational upper and lower bounds on ζ_n often enable us to decide whether a complex scattering system has a certain number of bound states or resonances in some region in the energy or the strength variables. They also give upper and lower bounds on the radius of convergence of the series expansion which appears in the iteration method or in perturbation theory.

It is irrelevant for our purpose whether $\mathcal{H}^{(1)}$ is a positive or a negative operator, and thus we assume $\mathcal{H}^{(1)}<0$ in the following discussion. The strength eigenvalue problem is

$$[\mathcal{H}^{(0)}-E+\zeta_n^{-1}\mathcal{H}^{(1)}]|\zeta_n\rangle=0,\qquad\text{(C1)}$$

with the normalization

$$\langle\zeta_n|\mathcal{H}^{(1)}|\zeta_m\rangle=-\delta_{nm}.\qquad\text{(C2)}$$

(C1) is the familiar form

$$(QE-\mathcal{H}^{(0)})^{-1}\mathcal{H}^{(1)}|\zeta_n\rangle=\zeta_n|\zeta_n\rangle,\qquad\text{(C3)}$$

which appears in the usual iteration procedure such as (5.13).

[14] H. A. Bethe and E. E. Salpeter, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 35, p. 344.

It is essential to note that, from the discreteness of the spectrum of the operators $\mathcal{H}$ and $\mathcal{H}^{(0)}$ for the given energy E below the threshold for new channels, ζ_n^{-1} is *bounded from below* with

$$0<\zeta_0^{-1}\leqslant\zeta_1^{-1}\leqslant\cdots. \tag{C4}$$

That is, the operator $\mathcal{H}$ has been constructed such that the negative part of the spectrum of $(\mathcal{H}-EQ)$ is *discrete*, and the interaction operator $\mathcal{H}^{(1)}$ does not change the locations of the thresholds. Therefore we can treat $(\mathcal{H}^{(0)}-EQ)$ exactly the same way as in the bound state problem, as far as its spectral structure is concerned.

(i) The upper bound on ζ_0^{-1} can be obtained trivially from (C1) and is of the form

$$\zeta_{0t}^{-1}=\frac{(\zeta_{0t}|[\mathcal{H}^{(0)}-EQ]|\zeta_{0t})}{(\zeta_{0t}|-\mathcal{H}^{(1)}|\zeta_{0t})}\geqslant\zeta_0^{-1}. \tag{C5}$$

Similarly, if we are interested in obtaining upper bounds on the higher states as well, then we can apply the Hylleraas-Undheim theorem and by diagonalizing the matrix $(\xi_t|[\mathcal{H}^{(0)}-EQ]|\xi_t)$ with the vector trial function $|\xi_t)$ which contains M terms we have

$$\zeta_{nt}^{-1}\geqslant\zeta_n^{-1},\quad \text{for } n=0,1,\cdots,N, \tag{C6}$$

with $N\leqslant M+1$. The condition that the eigenvalues of $\mathcal{H}$ and $\mathcal{H}^{(0)}$ given by $\mathcal{E}_n{}^Q$ and $\mathcal{E}_n{}^{(0)}$, respectively, are such that

$$\mathcal{E}_n{}^Q,\quad \mathcal{E}_n{}^{(0)}>E,\quad \text{for all } n, \tag{C7}$$

implies that

$$\zeta_n<1,\quad \text{for all } n, \tag{C8}$$

(C8) is just the condition of convergence of the iteration series (5.15). Thus, it follows from (C5) that if $\mathcal{H}^{(1)}<0$ and $1<\zeta_{0t}\leqslant\zeta_0$, then we are sure that the series diverges.

(ii) The lower bounds also follow readily by an analogous procedure used earlier in Sec. III. We consider a positive definite quantity

$$I=\left(\zeta_{0t}\left|\left[\mathcal{H}^{(0)}-E+\frac{\mathcal{H}^{(1)}}{\zeta_{0t}}\right][-\mathcal{H}^{(1)}]^{-1}\times\left[\mathcal{H}^{(0)}-E+\frac{\mathcal{H}^{(1)}}{\zeta_{0t}}\right]\right|\zeta_{0t}\right). \tag{C9}$$

Expanding $|\zeta_{0t})$ in the form

$$|\zeta_{0t})=\sum_{n=0}^{\infty}a_{nt}|\zeta_n\rangle, \tag{C10}$$

we have

$$I=\sum_{n=0}^{\infty}a_{nt}{}^2\left(\frac{1}{\zeta_{0t}}-\frac{1}{\zeta_n}\right)^2(\zeta_n|-\mathcal{H}^{(1)}|\zeta_n). \tag{C11}$$

Firstly, if

$$\zeta_{0t}^{-1}<\tfrac{1}{2}(\zeta_0^{-1}+\zeta_1^{-1}), \tag{C12}$$

then we get

$$I\geqslant\left(\frac{1}{\zeta_{0t}}-\frac{1}{\zeta_0}\right)^2(\zeta_{0t}|-\mathcal{H}^{(1)}|\zeta_{0t}). \tag{C13}$$

With the value ζ_{0t} chosen to satisfy $\zeta_{0t}^{-1}>\zeta_0^{-1}$ as can be obtained by an upper bound calculation we finally have[15]

$$1/\zeta_0\geqslant 1/\zeta_{0t}-[I/(\zeta_{0t}|-\mathcal{H}^{(1)}|\zeta_{0t})]^{1/2}. \tag{C14}$$

On the other hand, again from (C11), we have

$$I\geqslant(\zeta_{0t}^{-1}-\zeta_0^{-1})(\zeta_1^{-1}-\zeta_{0t}^{-1})(\zeta_{0t}|-\mathcal{H}^{(1)}|\zeta_{0t}), \tag{C15}$$

if

$$\zeta_0^{-1}<\zeta_{0t}^{-1}<\zeta_1^{-1}. \tag{C16}$$

Therefore we also get the lower bound

$$\zeta_0^{-1}\geqslant\zeta_{0t}^{-1}-\frac{I\zeta_1\zeta_{0t}}{(\zeta_{0t}-\zeta_1)(\zeta_{0t}|-\mathcal{H}^{(1)}|\zeta_{0t})}. \tag{C17}$$

The forms given by (C14) and (C17) are the analog of the formulas by Stevenson-Crawford and Temple, respectively, for the bound state problem.

The discussion given above can also be carried out in terms of the energy eigenvalue problem for the operators $\mathcal{H}$ and $\mathcal{H}^{(0)}$, although the argument is indirect. For the lowest state of $\mathcal{H}$, we have

$$\mathcal{E}_{0L}{}^Q<\mathcal{E}_0{}^Q<\mathcal{E}_{0U}{}^Q, \tag{C18}$$

with

$$\mathcal{E}_{0U}{}^Q=(Q\Phi_{0t}{}^Q|\mathcal{H}|Q\Phi_{0t}{}^Q)(Q\Phi_{0t}{}^Q|Q\Phi_{0t}{}^Q)^{-1},$$

$$\mathcal{E}_{0L}{}^Q=\mathcal{E}_{0U}{}^Q-J(\mathcal{E}_1{}^Q-\mathcal{E}_{0U}{}^Q)^{-1},$$

$$\mathcal{E}_0{}^Q<\mathcal{E}_{0U}{}^Q<\mathcal{E}_1{}^Q,$$

or,

$$\mathcal{E}_{0L}{}^Q=\mathcal{E}_{0U}{}^Q-J^{1/2}$$

$$\mathcal{E}_{0U}{}^Q<\tfrac{1}{2}(\mathcal{E}_0{}^Q+\mathcal{E}_1{}^Q),$$

where

$$J=(Q\Phi_{0t}{}^Q|\mathcal{H}^2|Q\Phi_{0t}{}^Q)-(Q\Phi_{0t}{}^Q|\mathcal{H}|Q\Phi_{0t}{}^Q)^2.$$

The upper bounds on the higher states can also be obtained using the Hylleraas-Undheim theorem.

Thus, if we carry out the calculation for $\mathcal{H}$ and $\mathcal{H}^{(0)}$ and obtain the various bounds such that, for example, the inequality

$$\mathcal{E}_{0U}{}^Q\leqslant E\leqslant\mathcal{E}_{0L}{}^{(0)}$$

holds, then the series such as (5.13) involving the kernel $(QE-\mathcal{H}^{(0)})^{-1}\mathcal{H}^{(1)}$ will surely be divergent.

Finally, we give an alternate expression for Δ using the eigenfunctions and the eigenvalues of the strength eigenvalue problem. Diagonalizing the $m\times m$ matrix $(\zeta_t|\mathcal{H}^{(0)}-EQ|\zeta_t)$ with the normalization given by (C2), we have

$$\Delta\leqslant\Delta_U, \tag{C19}$$

with

$$\Delta_U=\sum_{n=0}^{m}(1-\zeta_{nt})^{-1}(\zeta_{nt}|R_0)^2.$$

[15] See for example, L. M. Delves, Nucl. Phys. **45**, 443 (1963).