Remarks on Variational Bounds in Scattering Theory*

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The lower variational bound on the eigenphase shifts obtained by Sugar and Blankenbecler (SB) is shown to be formally equivalent to the upper variational bound $(\mathbf{K}^{-1})_{up}$ on the inverse of the reactance matrix $\mathbf{K}^{-1}$ that had been obtained earlier. By formally equivalent we mean that if the identical trial function is used in the two formulations, the eigenphase shifts contained in $(\mathbf{K}^{-1})_{up}$ are identical with those determined by the SB formulation. A still more recent variational bound by Rosenberg (R) is shown to be identical, for most purposes, to the SB result, and therefore also formally equivalent to the original variational bound. The SB and R approaches may nevertheless have certain advantages, since they suggest different actual numerical procedures. A lower variational bound on $\mathbf{K}^{-1}$ is obtained by means of the SB technique for determining upper bounds on the eigenphase shifts.

1. INTRODUCTION

THE first variational bounds derived in scattering theory were for the case of zero-incident relative kinetic energy for which single-channel elastic scattering is the only possible process. If the two systems cannot form a bound state, the expression that represents an upper variational bound on the scattering length[1] is exactly the same as one of the expressions obtained in a standard variational calculation. (Thus, with no additional labor, we can pass judgment on the relative merits of two such calculations, the lower number being the better one.) If the two systems can form a known number N_B of bound states, the upper variational bound on the scattering length requires the evaluation of N_B additional integrals, but the calculation is really equivalent to a standard variational calculation nonetheless.[2] The formulation has been applied to a number of atomic and nuclear scattering problems.

The formulation has been extended to include nonzero incident kinetic energies. The essential feature for zero and nonzero energies is the existence of a potential, which can be weak *or* strong. From the computational and from the formal point of view, however, the situation is much more complicated for an incident kinetic energy different from zero. Firstly, two different kinds of results were originally obtained, and under slightly different conditions. (We will return to the conditions later.) Lower bounds were obtained on the eigenphase shifts,[3] while upper variational bounds were obtained on the inverse $\mathbf{K}^{-1}$ of the reactance matrix $\mathbf{K}$.[4] (We use the word "bound" when the method generates one number which represents a bound on some quantity. We use the expression "variational bound" when the method generates not a numerical bound but a variational bound containing variational parameters which enable one not only to improve the variational bound but to improve it monotonically until, at least in principle, the variational bound assumes the exact value.) Secondly, for nonzero incident energies variational bound calculations are appreciably more difficult than standard variational calculations and every effort should be made to find new variational bounds or to improve the calculational techniques required for the evaluation of the original variational bound.

Recently, Sugar and Blankenbecler[5] derived upper and lower variational bounds on the eigenphase shifts. They were exceedingly gracious in acknowledging the use of some results of the earlier work, but they were under the impression that their lower variational bound on the eigenphase shifts was independent of the earlier upper variational bound on $\mathbf{K}^{-1}$. It is one of the main purposes of this article to show that, on the contrary, these two variational bound formulations are, in a sense to be described, formally identical.

It is very much simpler to obtain an upper variational bound on a discrete energy eigenvalue of a system than a lower variational bound. Correspondingly, it is always very much simpler to obtain one variational bound than the other on scattering parameters. The simpler variational bound to obtain is the upper one on the scattering length, the lower one on phase shifts and on eigenphase shifts, and the upper one on the inverse of the reactance matrix. Sections 2 and 3 are concerned with the "simple" variational bound, while Sec. 4 is concerned with the opposite, more difficult, variational bound.

2. LOWER VARIATIONAL BOUNDS ON THE EIGENPHASE SHIFTS

The starting points for the determination of a bound for nonzero incident kinetic energy[3] are the equivalent one-body equation[6]

$$P[H+HQG^{Q}QH-E]P\Psi=0\,, \qquad (2.1)$$

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[6] H. Feshbach, Ann. Phys. (N. Y.) **5**, 357 (1958); **19**, 287 (1962).

and the (numerically solvable) approximation equation

$$P[H-E]P\Psi^P=0. \tag{2.2}$$

[The notation is that of Refs. 3 and 4; we will not rederive most of the results but will simply summarize those that are relevant for our present purposes. Furthermore, we will for simplicity assume that the incident particle is distinguishable. (It is then possible to replace PHQ by PVQ, where V is the interaction between the incident particle and the target particles, but we will not do so.) The case of identical particles follows with entirely trivial modifications.] H is the full Hamiltonian. P is a projection operator on to all target states associated with open channels (P could include some closed channels in addition, but to simplify the discussion we will assume that it does not); $Q=1-P$, and $E=E_{T0}+E'$, with E the total energy of the system, E_{T0} the target ground-state energy, and E' the incident kinetic energy. G^Q, which is not normally calculable, is formally defined by

$$G^Q\equiv Q[Q(E-H)Q]^{-1}Q \tag{2.3}$$

and by appropriate boundary conditions. It is also useful to introduce the (numerically) *calculable* Green's function G^P defined by

$$G^P\equiv P[P(E-H)P]^{-1}P$$

and by appropriate boundary conditions. When P contains only one open channel, Eq. (2.2) corresponds to an approximation in which the target is fixed in its ground state and the approximation is then normally referred to as the static approximation. When P contains more than one open channel, Eq. (2.2) is often referred to as the close-coupling approximation equation.

The *continuous* spectrum of QHQ begins at the energy $E_{\rm cl}$ of the lowest closed channel. $E_{\rm cl}$ could be the energy of the lowest target state associated with a closed channel or it could be the energy associated with a pickup process, but in any event we have $E_{\rm cl}>E$. If QHQ does not have any *discrete* eigenvalues below E, which will often be the case, the inequality

$$Q(E-H)Q<0 \tag{2.4}$$

follows. Let us *assume* this inequality to be satisfied.

It is an immediate consequence that

$$G^Q<0, \tag{2.5}$$

and, since QHP is the adjoint of PHQ, that

$$\Gamma\equiv(PHQ)G^Q(QHP)<0. \tag{2.6}$$

On comparing Eqs. (2.1) and (2.2), we see that the effective interaction between the incident particle and the target is more negative for the true problem than it is for the static or close-coupling approximation. (In the true problem, the target can better adapt itself to the influence of the incoming particle since it can be virtually excited to target states associated with closed channels.) The monotonicity theorem immediately provides us with the sought-for bounds. With η_i and $\eta_i{}^P$ the ordered eigenphase shifts, we have

$$\eta_i>\eta_i{}^P, \quad 1\leq i\leq N^P, \tag{2.7}$$

where N^P is the number of open channels. Here and elsewhere, it will always be understood that some given total angular momentum is under consideration.

[Contrary to the impression often given in the literature, it is very difficult for scattering by a compound system to give an absolute definition of the phase shift, that is, a definition which fixes the multiple of π, which is calculationally meaningful. Inequality (2.7) is formally meaningless without such a definition. From the practical point of view, however, inequality (2.7) can be very helpful. This whole question is discussed in some detail in Ref. 3. All phase-shift inequalities in the present paper will be given this "practical" interpretation.]

Sugar and Blankenbecler[5] start from the same one-body equation (2.1) and from the same assumed inequality (2.4) but arrive at an improved result. Instead of simply saying that $G^Q<0$ and therefore that $\Gamma<0$, they construct an improved variational upper bound on G^Q and therefore on Γ, and therefore ultimately a variational lower bound on the η_i. Thus, it follows from Schwarz's theorem for any negative-definite Hermitian operator D which has a right inverse and for any function f_1 which may have to satisfy certain boundary conditions but which is otherwise arbitrary that

$$D\leq\frac{Df_1\rangle\langle f_1D}{\langle f_1|D|f_1\rangle}\leq 0;$$

therefore, operating with D^{-1} on the right, taking the Hermitian adjoint, and then operating with D^{-1} on the right again, it follows that

$$\frac{1}{D}\leq\frac{f_1\rangle\langle f_1}{\langle f_1|D|f_1\rangle}\leq 0.$$

We can therefore set D equal to $Q(E-H)Q$, and obtain a variational upper bound on G^Q. More generally, introducing the set of trial functions f_j, with j running from 1 to N, which vanish asymptotically but which are otherwise arbitrary, it also follows trivially from the Schwarz inequality that

$$\frac{1}{D}\leq\sum_{j,k}|f_j\rangle(\mathbf{D}^{-1})_{jk}\langle f_k|\leq 0, \tag{2.8}$$

where the matrix $\mathbf{D}$ has elements $\langle f_j|D|f_k\rangle$. Introducing the $1\times N$ *row* vector $|\mathbf{f}\rangle$ with elements which are the functions f_j,

$$|\mathbf{f}\rangle=(|f_1\rangle|f_2\rangle\cdots|f_N\rangle),$$

and the $N\times 1$ *column* vector

$$\langle \mathbf{f}| = \begin{bmatrix} \langle f_1| \\ \vdots \\ \langle f_N| \end{bmatrix},$$

the inequality (2.8) can be rewritten as

$$\frac{1}{D} \leq |\mathbf{f}\rangle\langle \mathbf{f}|D|\mathbf{f}\rangle^{-1}\langle \mathbf{f}| \leq 0. \tag{2.9}$$

(Note that with the somewhat unusual form of $\langle \mathbf{f}|$ and $|\mathbf{f}\rangle$ above, introduced to avoid the continual use of a transpose, entities such as $\langle \mathbf{f}|D|\mathbf{f}\rangle$ are not numbers but matrices.) Once again setting D equal to $Q(E-H)Q$, we arrive at

$$G^Q \leq |\mathbf{f}\rangle\mathbf{A}^{-1}\langle \mathbf{f}| \equiv G_S{}^Q \leq 0, \tag{2.10}$$

where $\mathbf{f}$ is to be chosen to lie in Q space, and where the matrix $\mathbf{A}$ is defined by

$$\mathbf{A} \equiv \langle \mathbf{f}|Q(E-H)Q|\mathbf{f}\rangle. \tag{2.11}$$

(As opposed to the purely formal if perfectly well-defined operator G^Q, the operator $G_S{}^Q$ defined by (2.10) is in an immediately usable form.) We immediately obtain the variational bound

$$\Gamma \equiv (PHQ)G^Q(QHP) \leq (PHQ)G_S{}^Q(QHP) \leq 0. \tag{2.12}$$

On introducing the approximate equivalent one-body problem defined by

$$P[H+HQG_S{}^QQH-E]P\Psi_S = 0, \tag{2.13}$$

with associated ordered eigenphase shifts η_{Si}, the lower variational bounds

$$\eta_i \geq \eta_{Si} \geq \eta_i{}^P, \quad 1 \leq i \leq N^P, \tag{2.14}$$

follow.[5] The η_{Si} are to be improved by varying the parameters contained in the functions f_j or by introducing additional functions.

The result, (2.14), therefore provides a lower variational bound on the η_i, whereas the original result, (2.7), provided only a lower bound on the η_i. (The original version corresponds to setting each of the f_j equal to zero.) It will, however, be interesting to compare the SB lower variational bound on the eigenphase shifts with the eigenphase shifts extracted from the original upper variational bound[4] on the inverse $\mathbf{K}^{-1}$ of the reactance matrix $\mathbf{K}$. We will now do this.

3. UPPER VARIATIONAL BOUND ON THE INVERSE OF THE REACTANCE MATRIX

Let K^P and K_S be the reactance matrices associated with Eqs. (2.2) and (2.13), respectively. By manipulating these two equations in the canonical way, that is, multiplying each by the solution of the other, subtracting, and integrating, one obtains

$$\Delta_S \equiv \mathbf{a}^T[(\mathbf{K}_S)^{-1} - (\mathbf{K}^P)^{-1}]\mathbf{a} = \langle P\Psi^P|PHQ\mathbf{f}\rangle\mathbf{A}^{-1}\langle \mathbf{f}|QHP\Psi_S\rangle. \tag{3.1}$$

(As always, there appear the two wave functions and the difference in the corresponding potentials.) The components of the $N^P\times 1$ matrix $\mathbf{a}$ are arbitrary and appear in the specification of the boundary conditions assumed for $P\Psi^P$, for $P\Psi_S$, and for $P\Psi$. They are related to the amplitudes of the regular functions in the different open channels.

As noted earlier, we consider $P\Psi^P$ and G^P, which are defined by a set of N^P coupled equations, to be numerically determinable. Since $G_S{}^Q$, upon diagonalization, consists of a finite number of separable terms—that is why we used the subscript S in $G_S{}^Q$—any quantity associated with Eq. (2.13) can be obtained. Thus, we rewrite Eq. (2.13) as the integral equation

$$\begin{aligned} P\Psi_S &= P\Psi^P + G^PPHQG_S{}^QQHP\Psi_S \\ &= P\Psi^P + G^PPHQ|\mathbf{f}\rangle\mathbf{A}^{-1}\langle \mathbf{f}|QHP\Psi_S\rangle. \end{aligned} \tag{3.2}$$

Multiplying through by $\langle \mathbf{f}|QHP|$, we find

$$\langle \mathbf{f}|QHP\Psi_S\rangle = [\mathbf{1} - \langle \mathbf{f}|QHPG^PPHQ|\mathbf{f}\rangle\mathbf{A}^{-1}]^{-1} \times \langle \mathbf{f}|QHP\Psi^P\rangle. \tag{3.3}$$

Substituting into Eq. (3.1), we have our explicit expression

$$\Delta_S = \langle P\Psi^P|PHQ\mathbf{f}\rangle[\mathbf{A} - \langle \mathbf{f}|QHPG^PPHQ|\mathbf{f}\rangle]^{-1} \times \langle \mathbf{f}|QHP\Psi^P\rangle. \tag{3.4}$$

Introducing the operator $\mathfrak{C}$, which crops up regularly in this topic, defined by

$$Q(\mathfrak{C}-E)Q \equiv Q(H+HG^PH-E)Q, \tag{3.5}$$

and using Eq. (2.11), we immediately obtain

$$\Delta_S = \langle P\Psi^P|PHQ\mathbf{f}\rangle[\langle \mathbf{f}|Q(E-\mathfrak{C})Q|\mathbf{f}\rangle]^{-1} \times \langle \mathbf{f}|QHP\Psi^P\rangle. \tag{3.6}$$

Since $\mathbf{a}$ is arbitrary, one can extract $\mathbf{K}_S{}^{-1}$ from (3.6).

Let us now introduce the quantity Δ associated with the exact and static equations, (2.1) and (2.2),

$$\Delta \equiv \mathbf{a}^T[\mathbf{K}^{-1} - (\mathbf{K}^P)^{-1}]\mathbf{a}. \tag{3.7}$$

It does *not* follow from the above discussion that Δ_S provides a variational bound (or even a bound) on Δ, nor that $\mathbf{K}_S{}^{-1}$ provides a variational bound (or even a bound) on $\mathbf{K}^{-1}$; the elements of $\mathbf{K}^{-1}$ involve trigonometric functions of the η_i in addition to mixing parameters and a bound on η_i does not provide a bound on a trigonometric function of η_i.

One *can* obtain an upper variational bound on Δ and therefore on $\mathbf{K}^{-1}$. It was shown[4] that Δ could be written as

$$\Delta = 2\langle Q\Psi_t|H|P\Psi^P\rangle + \langle Q\Psi_t|Q(\mathfrak{C}-E)Q|Q\Psi_t\rangle - \langle Q\Omega|Q(\mathfrak{C}-E)Q|Q\Omega\rangle, \tag{3.8}$$

where $\mathfrak{C}$ is defined by (3.5), where $Q\Psi_t$ is a trial function in closed channel space which must therefore vanish

asymptotically, and where $Q\Omega$ is the (unknown) difference function defined by

$$Q\Omega \equiv Q\Psi_t - Q\Psi .$$

$Q\mathcal{H}Q$ differs from QHQ by a potential term, and its continuous spectrum, as that of QHQ, will begin above E. It will often be the case that $Q\mathcal{H}Q$ does not have a discrete spectrum, which is sufficient though not necessary to guarantee that

$$Q(E-\mathcal{H})Q<0. \tag{3.9}$$

Let us *assume* this to be the case. It follows immediately, looking at the boundary conditions satisfied by $Q\Omega$, that

$$\Delta \leq \Delta_{\rm up} \equiv 2\langle Q\Psi_t | H | P\Psi^P\rangle + \langle Q\Psi_t | Q(\mathcal{H}-E)Q | Q\Psi_t\rangle . \tag{3.10}$$

Since **a** is arbitrary, one can extract an upper variational bound on $\mathbf{K}^{-1}$ from (3.10),

$$\mathbf{K}^{-1} \leq (\mathbf{K}^{-1})_{\rm up} .$$

Taking $Q\Psi_t$ to be of the form

$$|Q\Psi_t\rangle = \Sigma_j c_j |f_j\rangle \equiv |\mathbf{f}\rangle \mathbf{C} , \tag{3.11}$$

(as defined earlier, $|\mathbf{f}\rangle$ is a *row* vector while $\mathbf{C}$ is a column vector in the parameter space), with the same set of functions f_j as chosen previously, and minimizing the right-hand side of (3.10) with respect to the linear variational parameters c_j, one finds that $\Delta_{\rm up}$ reduces to Δ_S, defined by (3.6). We thus have

$$\Delta \leq \Delta_{\rm up} = \Delta_S . \tag{3.12}$$

We also have

$$K^{-1} \leq (K^{-1})_{\rm up} = K_S^{-1} . \tag{3.13}$$

We can now summarize the formal results as follows. If inequality (2.4) is satisfied, the "static" or "close coupling" eigenphase shift η_i^P provides a lower bound on η_i; better still, η_{Si} provides a lower variational bound on η_i. If the *different* inequality (3.9) is satisfied, $\Delta_{\rm up}$ provides a variational bound on Δ. Finally, assume that *both* inequalities are satisfied, which will often be the case, and that the same functions f_j are used in the determination of the lower variational bounds η_{Si} and in the determination of the upper variational bound $(\mathbf{K}^{-1})_{\rm up}$. It follows from our discussion that the eigenphase shift estimates (modulo π) extracted from $(\mathbf{K}^{-1})_{\rm up}$ are *exactly* the η_{Si}. It is in this sense that the two variational bounds are formally the same.

The exact agreement of the two variational bounds may seem somewhat remarkable, especially since they begin with the assumption of different inequalities, (2.4) and (3.9). The agreement can be made more reasonable by a consideration of Green's functions. Thus, Eq. (2.1) represents the uncoupled equation for $P\Psi$. The corresponding uncoupled equation for $Q\Psi$ is given by

$$Q[\mathcal{H}-E]Q\Psi = -QHP\Psi^P , \tag{3.14}$$

(The inhomogeneous term contains $P\Psi^P$, *not* $P\Psi$.) Introducing the Green's function $\mathcal{G}^Q$ defined by

$$Q[\mathcal{H}-E]Q\mathcal{G}^Q = -Q \tag{3.15}$$

and by appropriate boundary conditions, we have

$$Q\Psi = \mathcal{G}^Q QHP\Psi^P . \tag{3.16}$$

In addition to the forms of Δ that were used in the derivation of (3.8),

$$\Delta = (P\Psi^P, PHQ\Psi) \tag{3.17}$$

and

$$\Delta = -(Q\Psi, [\mathcal{H}-E]Q\Psi) , \tag{3.18}$$

we can therefore also write

$$\Delta = (QHP\Psi^P, \mathcal{G}^Q QHP\Psi^P) . \tag{3.19}$$

$\mathcal{G}^Q$ is a formidable operator, but if (3.9) is satisfied, it can be bounded in exactly the same way[5] that G^Q was. With $\mathcal{H}$ defined by (3.5), we then have, in analogy with (2.10),

$$\mathcal{G}^Q \leq |\tilde{\mathbf{f}}\rangle \mathfrak{A}^{-1} \langle \tilde{\mathbf{f}}| \equiv \mathcal{G}_S^Q , \tag{3.20}$$

where $|\tilde{\mathbf{f}}\rangle$ is an arbitrary $1\times N$ *row* vector in Q space and where

$$\mathfrak{A} \equiv \langle \tilde{\mathbf{f}} | Q(E-\mathcal{H})Q | \tilde{\mathbf{f}}\rangle . \tag{3.21}$$

It follows immediately that

$$\Delta \leq \langle QHP\Psi^P | \tilde{\mathbf{f}}\rangle \mathfrak{A}^{-1} \langle \tilde{\mathbf{f}} | QHP\Psi^P\rangle \equiv \Delta'_{\rm up} . \tag{3.22}$$

If we choose $|\tilde{\mathbf{f}}\rangle = |\mathbf{f}\rangle$, we find that

$$\Delta'_{\rm up} = \Delta_{\rm up} = \Delta_S . \tag{3.23}$$

This remarkably simple connection between $\Delta'_{\rm up}$ and Δ_S for $|\tilde{\mathbf{f}}\rangle$ chosen equal to $|\mathbf{f}\rangle$, and the not unrelated formal equivalence of the two variational bounds, have their roots in the following connection between G_S^Q and $\mathcal{G}_S^Q$, for $|\tilde{\mathbf{f}}\rangle$ chosen equal to $|\mathbf{f}\rangle$. The exact Green's functions G^Q and $\mathcal{G}^Q$ satisfy the relationship

$$\mathcal{G}^Q = G^Q + \mathcal{G}^Q QHPG^P PHQG^Q . \tag{3.24}$$

This follows from the defining relations, (2.3) and (3.15). We will now show that $\mathcal{G}_S^Q$ and G_S^Q satisfy an analogous equation,

$$\mathcal{G}_S^Q = G_S^Q + \mathcal{G}_S^Q QHPG^P PHQG_S^Q . \tag{3.25}$$

Because of the separability of G_S^Q, as given by (2.10), $\mathcal{G}_S^Q$ as defined by (3.25) can be obtained explicitly. Substituting for G_S^Q from (2.10), we need merely multiply (3.25) on the right by $QHPG^PPHQ|\mathbf{f}\rangle$, solve for $\mathcal{G}_S^Q QHPG^PPHQ|\mathbf{f}\rangle$, and substitute back into (3.25). We then find

$$\mathcal{G}_S^Q = |\mathbf{f}\rangle [\langle \mathbf{f}| Q(E-\mathcal{H})Q|\mathbf{f}\rangle]^{-1} \langle \mathbf{f}| , \tag{3.26}$$

which, with $|\tilde{\mathbf{f}}\rangle = |\mathbf{f}\rangle$, agrees with (3.20). Thus, to go from G_S^Q to $\mathcal{G}_S^Q$, we need merely replace H by $\mathcal{H}$. The presence of the *same* function $|\mathbf{f}\rangle$ in both Green's functions is the origin of the various simplifications noted above.

We have up to this point restricted ourselves to the case for which $Q(\mathcal{H}-E)Q$ and $Q(H-E)Q$ have only continuous spectra, but the method of obtaining a variational bound when there is a known number of discrete eigenvalues has been available for some time.[2,4] The formal equivalence of the two formulations can readily be extended to include the case when the number of discrete eigenvalues of $Q(\mathcal{H}-E)Q$ and of $Q(H-E)Q$ is the *same*.

Very recently, a third version of variational bounds has appeared.[7] Rosenberg showed that if (2.4) is satisfied, the ordered eigenphase shifts of the approximate equivalent one-body problem

$$\omega_t^\dagger(H-E)\omega_t\Psi_R=0\,, \tag{3.27}$$

where

$$\omega_t\equiv P+G_t^Q QHP \tag{3.28}$$

with G_t^Q an arbitrary approximation to G^Q, provides lower variational bounds on the eigenphase shifts of the original problem. For the reasonable and useful (but not necessary) choice $G_t^Q=G_S^Q$, with G_S^Q defined by (2.10), it is trivial to check that (3.27) reduces to (2.13).

More generally, let us consider the choice

$$G_t^Q=\Sigma_{j,k}|f_j\rangle d_{jk}\langle f_k|=|\mathbf{f}\rangle\mathbf{D}\langle\mathbf{f}|\,, \tag{3.29}$$

where the matrix $\mathbf{D}$ is to be symmetric but is as yet otherwise unspecified. Eq. (3.27) then becomes

$$P[H-E+H|\mathbf{f}\rangle(2\mathbf{D}-\mathbf{DAD})\langle\mathbf{f}|H]P\Psi_R=0 \tag{3.30}$$

with $\mathbf{A}$ defined by (2.11). The best possible choice of $\mathbf{D}$ is that which makes $2\mathbf{D}-\mathbf{DAD}$ an extremum. This is readily seen to be $\mathbf{D}=\mathbf{A}^{-1}$, in which case $2\mathbf{D}-\mathbf{DAD}$ reduces to $\mathbf{A}^{-1}$ and (3.30) reduces to (2.13). We thus see that for the very reasonable and quite wide class of choices encompassed by (3.29), Rosenberg's formulation is equivalent to that of Ref. 5 and therefore in turn is formally equivalent to that of Ref. 4.

Since the dimensionality of $|\mathbf{f}\rangle$ in (3.29) will necessarily be finite, the form (3.29) is not quite completely general. Thus, one might approximate the nonlocal operator G^Q by an approximation G_t^Q which is local and which could only be expressed in the form of (3.29) by an infinite sum.

It may be of interest to derive Rosenberg's result in a somewhat simpler fashion than that used originally. For a positive definite A, it follows immediately if $A^{1/2}$ has a left and a right inverse [this latter requirement is not necessary to obtain (3.31)] from

$$(1-A^{1/2}\beta A^{1/2})^2\geq 0\,,$$

where β is arbitrary, that

$$1/A\geq 2\beta-\beta A\beta\,. \tag{3.31}$$

Rosenberg's result follows from using (3.31), with $A=Q(H-E)Q$, in Eq. (2.1).

[7] L. Rosenberg, Phys. Rev. **138**, B1343 (1965).

We will not use the result, but because it might prove fruitful, we record the result

$$\mathcal{G}^Q\equiv Q\frac{1}{Q(E-\mathcal{H})Q}Q=Q\frac{1}{E-H}Q. \tag{3.32}$$

This result is proved in Appendix B of Ref. 3.

4. THE *OPPOSITE* BOUND

As noted earlier, it is far more difficult to obtain upper than lower variational bounds on the eigenphase shifts and lower than upper variation bounds on $\mathbf{K}^{-1}$. The results that have been obtained for the opposite more difficult bounds (or variational bounds) are much less useful and the discussion will be much briefer.

Under reasonably general conditions, it is possible to obtain the opposite bound by obtaining a simple (if possibly crude) *numerical* lower bound G^Q on G^Q.[8] Thus, let us assume that we can find an energy E^Q such that

$$QHQ\geq E^Q>E. \tag{4.1}$$

This may be possible if (2.4) is valid. If QHQ has no discrete spectrum, we can choose $E^Q=E_{\rm cl}$. If QHQ has a discrete spectrum but the lowest eigenvalue lies above E, we can set E^Q equal to that lowest eigenvalue. If that lowest eigenvalue lies below E, there are a number of things that can be done, at least in principle, one of which is to include more states in P space, and therefore fewer in Q space. In any event, assuming that we can find an E^Q satisfying (4.1), we immediately have

$$G^Q\equiv Q[Q(E-H)Q]^{-1}Q\geq Q(E-E^Q)^{-1}\equiv G_L^Q\,. \tag{4.2}$$

The solution of the equation

$$P[H+(E-E^Q)^{-1}HQH-E]P\Psi''=0 \tag{4.3}$$

then provides the other bound, the upper bound on the η_i.[8] Though the approach is not always applicable, and though the upper bound, even when applicable, is of limited accuracy, (4.3) does at least have the virtue, when applicable, of being sufficiently simple that one can actually obtain numerical bounds. (PHQ reduces to PVQ for a distinguishable incident particle, and a comparable simplification occurs for an indistinguishable incident particle. The essential point is that the difficult kinetic energy operators vanish when between P and Q.)

An approach which is in principle much superior, in that it supplies a variational upper bound on the η_i, is available.[5] Assuming inequality (4.1) to be satisfied, it can be shown that

$$G^Q\geq(E-E^Q)^{-1}\times\{1+F|\mathbf{p}\rangle[\langle\mathbf{p}|F(1-F)|\mathbf{p}\rangle]^{-1}\langle\mathbf{p}|F\}\equiv G_\sigma^Q\,, \tag{4.4}$$

[8] L. Spruch, in *Few Nucleon Problems, Ninth Summer Meeting of Yugoslav Physicists, Hercegnovi,* edited by M. Cerineo (Federal Nuclear Energy Commission of Yugoslavia, Belgrade, 1964).

where $|\mathbf{p}\rangle$ is an arbitrary $1\times N$ matrix and where

$$F\equiv Q(H-E^Q)Q/(E-E^Q). \tag{4.5}$$

The solution of the equation obtained by replacing G^Q in (2.1) by $G_\sigma{}^Q$,

$$P[(H-E)+HQG_\sigma{}^QQH]P\Psi_\sigma=0, \tag{4.6}$$

provides variational upper bounds on the eigenphase shifts. [Upper variational bounds were also obtained[5] when (2.4) is not satisfied, by the approximate "subtraction" of the discrete eigenvalues following the procedure of Refs. 2 and 4.]

Although this procedure is, in principle, of potentially unlimited accuracy, unfortunately, as is so often the case in formalisms for the difficult bound, it requires, because of the appearance of $\langle\mathbf{p}|F(1-F)|\mathbf{p}\rangle$, the evaluation of matrix elements of the square of H, and is therefore extremely difficult to use.

Extensions and generalizations along the lines of both of the above approaches are included in the contents of a recent paper,[9] but no truly general and practical approach is yet available.

(4.3) and (4.6) were based on the possibility of obtaining a numerical lower bound $G_L{}^Q$ on G^Q, and an operator lower variational bound $G_\sigma{}^Q$ on G^Q, respectively. Corresponding results can be obtained by considering $\mathcal{G}^Q$ rather than G^Q. These latter results are in some ways more useful since inequalities on trigonometric functions of phase shifts are normally more useful than inequalities on the phase shifts themselves.

Thus, if we can find an energy $\mathcal{E}^Q$ such that

$$Q\mathcal{H}Q\geq\mathcal{E}^Q>E, \tag{4.7}$$

which should be possible if (3.9) is valid, we have

$$\mathcal{G}^Q\equiv Q[Q(E-\mathcal{H})Q]^{-1}Q\geq Q(E-\mathcal{E}^Q)^{-1}. \tag{4.8}$$

It then follows from (3.19) that

$$\Delta\geq(E-\mathcal{E}^Q)^{-1}(QHP\Psi^P,QHP\Psi^P). \tag{4.9}$$

Correspondingly, if (3.9) is valid, a lower variational bound on Δ is obtained by utilizing the analogue of (4.4) and (4.5), namely,

$$\mathcal{G}^Q\geq(E-\mathcal{E}^Q)^{-1}\times\{1+\mathfrak{F}|\mathfrak{P}\rangle[\langle\mathfrak{P}|\mathfrak{F}(1-\mathfrak{F})|\mathfrak{P}\rangle]^{-1}\langle\mathfrak{P}|\mathfrak{F}\}\equiv\mathcal{G}_\sigma{}^Q, \tag{4.10}$$

where

$$\mathfrak{F}\equiv Q(\mathcal{H}-\mathcal{E}^Q)Q/(E-\mathcal{E}^Q). \tag{4.11}$$

We then have

$$\Delta\geq(QHP\Psi^P,\mathcal{G}_\sigma{}^QQHP\Psi^P). \tag{4.12}$$

As opposed to the situation for the "simple" bounds, there does not for the difficult bounds appear to be any elegantly simple connection between the approach based on the equivalent one-body equation (2.1) and the approach based on an analysis of Δ. Such connections are not to be expected since $\mathcal{G}_\sigma{}^Q$ and $G_\sigma{}^Q$ do not appear to satisfy the analog of (3.25).

We would like to mention that we have shown (to be published) that, as is intuitively reasonable, the adiabatic approximation can also be used to obtain the difficult opposite bound.

5. CONCLUSIONS

The *formal* equivalence of the Sugar-Blankenbecler lower variational bound on the eigenphase shifts (and, by and large, of the Rosenberg variational bound) with an earlier version[4] do not detract from their potential importance, for they suggest an alternative procedure for performing the necessary *numerical* calculations. The advantages and disadvantages of the different approaches will only become clear after many further numerical calculations have been performed. It may very well be, for example, that the relative merits of the various approaches depend upon how close the scattering energy is to a resonance.

We make one final observation. The equivalence between the SB and the original formulations was shown to be intimately related to the connection between G^Q and $\mathcal{G}^Q$ given by (3.24), or rather to the connection (3.25) between $G_S{}^Q$ and $\mathcal{G}_S{}^Q$, the approximations to G^Q and $\mathcal{G}^Q$, respectively. The SB formulation contains $G_S{}^Q$ which involves the matrix element of $Q(H-E)Q$, while the other formulation can be expressed in terms of $\mathcal{G}_S{}^Q$ which involves the matrix element of $Q(\mathcal{H}-E)Q$. Thus in one case the energy-independent operator H appears, while in the other case the energy-dependent operator $\mathcal{H}(E)$ appears. A comparison of the two is therefore reminiscent of a comparison of the Wigner-Eisenbud and Kapur-Peierls formulations of reaction theory. These latter formulations are clearly equivalent to one another since they are each exact. (The reminiscence would seem to be marred by the existence of a cutoff radius in the theory of nuclear reactions, a cutoff which does not appear in the variational bound expressions since they utilize the unified reaction theory of Feshbach[6] which does not intrinsically contain a cutoff radius. Such a radius can, however, be readily introduced into unified reaction theory by the appropriate choice of the projection operator, and the relationship between the Wigner-Eisenbud and Kapur-Peierls approaches has been considered by Feshbach[6] within the context of his unified theory.) The equivalence of the different formulations of variational bounds was by no means obvious since they are approximations to the exact results.

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[9] Y. Hahn, Phys. Rev. **139**, B212 (1965).