Variational Upper and Lower Bounds for Multichannel Scattering*

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Upper and lower variational bounds are given for all elements of the reaction matrix. These, in turn, lead to upper and lower bounds on the elastic and inelastic cross sections. We explicitly discuss two-particle scattering, coupled two-particle channels, and three-particle scattering situations, and our methods will work for any number of particles. Numerical examples are given, including phase shift bounds for s-wave electron-hydrogen scattering. It is hoped that this approach will lead to a tractable calculational scheme for strongly interacting relativistic particles.

I. INTRODUCTION AND MOTIVATION

THE single most striking fact in the theory of strong interactions is the difficulty of making reliable calculations. The only quantitative test of a theory so far has been the check that the forward pion-nucleon dispersion relations proposed by Goldberger[1] are satisfied by the experimental data.[2] The difficulties in performing calculations in relativistic theories which necessarily allow an infinite number of particles in virtual states are self-evident but probably not completely known.

There have been a number of approximate calculations which yield agreement with the data but it is not clear whether the agreement is due to the approximations made or to the physical model underlying the various calculations.

It is important to note that the approximations used to handle such problems arrange themselves into two distinct levels. The deep approximation is the restriction to a finite number of particles in intermediate states. This is a necessary step in order to handle the problem at all. The shallow approximations are made in extracting numbers from a theory after the number of particles has been restricted. These latter approximations can be tested, as we shall see, simply because the problem can be stated mathematically. It is our purpose here to develop techniques which allow one to calculate upper and lower bounds on certain physical parameters, for instance, the elastic phase shifts, after the number of particles considered has been made finite.

The type of approach to strong interaction physics that we are advocating is roughly as follows. Sum all Feynman graphs with N particles or less in intermediate states into a coupled system of Bethe-Salpeter[3] type equations. This defines a model theory of order N. Exact crossing symmetry is, of course, destroyed by this procedure; however, unitarity is satisfied in the N-particle sector. This coupled system predicts certain parameters, among which are the elastic phase shifts, and one then calculates a set of numbers $\delta_l(N)$.

The next state in the procedure is to increase N to $N+1$ and the new coupled system of equations written down with improved kernels which are crossing-symmetric to order $N+1$. These equations then yield the predictions $\delta_l(N+1)$. In principle, at least, this procedure is repeated ad infinitum, and one calculates all quantities of physical interest.

It is an interesting question whether or not the model phase shifts converge as one increases N, and if they do, whether or not they converge to the full relativistic theory values. These are deep questions and will not be discussed here.

The obvious difficulty here lies in extracting the phase shifts from such a complicated set of equations. While it is probably impossible to calculate the phase shifts exactly, it is our purpose here to develop methods which allow one to place simple upper and lower variational bounds on the phase shifts.

The use of Bethe-Salpeter equations in the above example is used only for illustrative purposes and because we are sure our procedures will work in such a case. We hope that we will be able to extend our bounds to scattering amplitudes defined by analyticity and unitarity requirements only. We have already extended some of our results to partial-wave dispersion relations and this will be discussed later.

In this paper we will develop methods which allow one to get bounds on phase shifts (much of what we do can be carried over directly to the eigenphase shifts) and elements of the K matrix for potential scattering. In a later paper, the more complicated Bethe-Salpeter case will be discussed.

In this paper we will need to study directly the effect of changing the potentials on the elastic phase shifts.[4] To that end, we must study explicit formulas for $\delta_l(E)$

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† John B. Putnam Junior Fellow, 1963–1964.
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[2] J. W. Cronin, Phys. Rev. **118**, 824 (1960).
[3] H. Bethe and E. Salpeter, Phys. Rev. **84**, 1232 (1951); M. Gell-Mann and F. E. Low, *ibid.* **84**, 350 (1951).
[4] This paper is an extension of the work reported by R. Blankenbecler, lectures given at the Scottish Summer School of Theoretical Physics, 1963 (unpublished).

and not just the equations which the Green's functions or T matrices satisfy. The Fredholm determinantal approach seems to be the simplest tool for this study. However, in order to carry out this discussion, we must demonstrate that solutions exist, and we must develop what seem to be slightly more general methods than used before.

The two-body problem has been discussed many times. Two important discussions, where previous references may be found, are due to Hunziker[5] and Newton,[6] who also discussed the coupled channel case. The general three-body problem has been discussed by Faddeev,[7] whose work was considerably extended by Lovelace.[8] Weinberg[9] has considered the N-body problem with an approach which is closer to our own discussions than the Faddeev-Lovelace approach.

These authors were more concerned with general questions of existence than with viable calculational schemes. These will be our main concern. The roots of our approach are to be found in the classic minimum variational method of Rayleigh-Ritz[10] and the interesting work of Bazley-Fox[11] on maximum variational methods. These authors deal only with eigenvalues whereas we will be mostly interested in the continuum problem. A generalization of the Bazley-Fox eigenvalue scheme so that it applies to any Hamiltonian will be presented. This will be needed in our discussion of the multichannel situation.

Undoubtedly the most important theoretical development in variational principles for the scattering of complicated systems has been the minimum principle developed by Spruch and collaborators,[12] as an extension and simplification of the work of Kato.[13] Our minimum principle works for all energies in the elastic region and is quite distinct from the Spruch approach.

As an illustration of our method, electron-hydrogen and positron-hydrogen scattering will be discussed, but detailed calculations will be presented only for the former problem. The theory of these processes has been thoroughly discussed in the literature. Those which bear some resemblance to the treatment given here are the works of Spruch[12] with the magnificent calculation of Schwartz,[14] and theory and calculations of Temkin,[15] and the optical potential approach of Watson and Mittleman.[16] The close-coupling approximation used by Burke and Schey[17] also has certain similarities. In this connection we would like to mention the excellent review article of Burke and Smith.[18]

Our work will involve the use of separable potentials and in that connection we should point out the work by Mitra[19] and the solvable stripping models of Amado.[20]

Finally, and most importantly, we note that our treatment can be extended to give upper and lower variational bounds on all elements of the reaction matrix. This result is based on the fact that we have developed *both* an upper and lower variational bound on the effective potential matrix for the many-channel situation. The bounds on the reactance matrix lead in turn to bounds on both elastic and inelastic cross sections.

In Sec. II, the problem of upper and lower bounds on phase shifts and eigenvalues is discussed for two-particle scattering. In Sec. III, some numerical examples are presented and an upper and lower bound on the value of the Regge trajectory at zero energy is worked out. Both the weak and strong coupling limit is examined.

In Sec. IV, the problem of coupled two-particle channels is taken up. In Sec. V, the three-body problem is formulated and bounds on the K matrix are given in terms of effective potentials. In Sec. VI, the problem of electron-hydrogen scattering is discussed and preliminary numerical results given. This is done as a test of the feasibility of our method in a complicated problem—one cannot hope to improve on the numerical results of Schwartz.[14] Section VII is devoted to a review of results.

II. SINGLE-CHANNEL POTENTIALS

A. Scattering

Before we can start on any discussion of multichannel and multiparticle scattering, the problem of two-particle scattering must be dealt with. We will treat this latter problem so as to bring out its close analogy to our later discussion of the more interesting problem of multiparticle scattering. Our point of departure is the Lippmann-Schwinger equation for the full Green's function g in the presence of a potential V,

$$g=G+GVg\equiv G+vg\,, \tag{1}$$

where G is the free Green's function, given formally by $(E-H_0+i\epsilon)^{-1}$. The T matrix can be introduced by

[5] W. Hunziker, Helv. Phys. Acta **34**, 593 (1961).
[6] R. Newton, J. Math. Phys. **1**, 319 (1960); **2**, 188 (1961).
[7] L. D. Faddeev, Zh. Eksperim i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)]; Dokl. Akad. Nauk SSSR **138**, 565 (1961); **145**, 301 (1962) [English transls.: Soviet Phys.—Doklady **6**, 384 (1961); **7**, 600 (1963)].
[8] C. Lovelace, lectures given at the Scottish Summer School in Theoretical Physics, 1963 (unpublished).
[9] S. Weinberg, Phys. Rev. **133**, B232 (1964); see also W. Hunziker (to be published).
[10] See any text on quantum mechanics.
[11] N. W. Bazley and D. W. Fox, Phys. Rev. **124**, 483 (1961).
[12] See, for example, Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **130**, 381 (1963).
[13] T. Kato, Phys. Rev. **80**, 475 (1950); Progr. Theoret. Phys. (Kyoto) **6**, 394 (1951).
[14] C. C. Schwartz, Phys. Rev. **124**, 1468 (1961).
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[16] K. M. Watson, Phys. Rev. **105**, 1388 (1957); M. H. Mittleman and K. M. Watson, *ibid.* **113**, 198 (1959); B. A. Lippmann, M. H. Mittleman, and K. M. Watson, *ibid.* **116**, 920 (1959).
[17] P. C. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).
[18] P. C. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962).
[19] A. N. Mitra, Phys. Rev. **127**, 1342 (1962).
[20] R. Amado, Phys. Rev. **132**, 485 (1963).

defining

$$g=G+GTG \tag{2}$$

or

$$T=V+VgV.$$

The formal solution of Eq. (1) is

$$g=(1-v)^{-1}G\equiv KG. \tag{3}$$

It is well known that Fredholm theory cannot be directly applied to the calculation of the resolvent K. The difficulty is that the Fredholm determinant, given by

$$\det(1-v)=\exp[\mathrm{Tr}\ln(1-v)], \tag{4}$$

does not exist for any local potential since $\mathrm{Tr}v$ is infinite. This disease can be cured in many ways. We will choose a method which can be extended to more complicated problems. Let us attempt to write the resolvent in the form

$$K=L[M(1-v)L]^{-1}M, \tag{5}$$

where L and M are arbitrary kernels. In order that (5) satisfy the Lippmann-Schwinger equation, we must require the existence of

(a) M^{-1}

and

$$\text{(b) } D=\det[M(1-v)L]. \tag{6}$$

These are quite weak restrictions on L and M. There are two choices of these kernels that lead to familiar forms of the determinant. If $M=1$, and $L=1+v$, then one finds

$$D=\det[1-vv].$$

This is equivalent to iterating Eq. (1) once as was done by Khuri.[21] If one chooses $M=1$ and $L=\exp(v)$, then

$$D=\exp\mathrm{Tr}[\ln(1-v)+v].$$

This corresponds to the prescription of Jost and Pais[22] and Baker.[23] It is equivalent to the replacement of $\mathrm{Tr}(v)$ by zero everywhere that it appears in the expansion of the ordinary determinant given by Eq. (4).

In order to prove that the determinant exists for physical energies and is an entire function of the coupling constant, let us reexamine D for the choice

$$L=\exp(v)M^{-1}.$$

Then

$$D=\det[\exp(v)\times(1-M^{-1}vM)],$$

and by direct manipulation (see Baker, Ref. 23) or use of Schwartz's inequality, we see that

$$|D|^2\leq\exp\mathrm{Tr}[(M^{-1}vM)(M^{-1}vM)^\dagger]\equiv\exp T,$$

where the dagger means Hermitian conjugation. Defining $F=(MM^\dagger)^{-1}$, we have

$$T=\mathrm{Tr}[FvF^{-1}v^\dagger].$$

The determinant D will be an entire function of the coupling constant if we can show that there exists an F which makes T finite. There are an infinite number of suitable operators; for example, if we choose to make F local in coordinate space, then T becomes

$$T=\frac{1}{(4\pi)^2}\int d^3rd^3r'\frac{F(r)}{|\mathbf{r}-\mathbf{r}'|^2}\frac{V^2(r')}{F(r')}\times\exp(-2\,\mathrm{Im}k|\mathbf{r}-\mathbf{r}'|). \tag{7}$$

There are many F's which make T finite even when $\mathrm{Im}k$ is zero. In fact, let us choose the local F which makes T a minimum (or at least stationary). We have for the change in T when we vary F

$$\delta T=\int d^3rd^3r'S(r,r')\left[\frac{\delta F(r)}{F(r')}-\frac{F(r)\delta F(r')}{F^2(r')}\right]V^2(r'),$$

where S is symmetric in r and r'. If r and r' are interchanged in the second term, then the requirement that the variation of T vanish leads to

$$F(r)=\pm V(r),$$

or

$$M=[\pm V(r)]^{-1/2}.$$

This is the optimum choice for a local $F(r)$ and is the operator advocated by Scadron, Weinberg, and Wright[24] to make the kernel of the Hilbert-Schmidt class for all energies on the physical sheet and its boundaries.

However, this is not the optimum choice for M if nonlocal operators are admitted. A simple choice is the separable operator.

$$M^{-1}=(\pm V)^{1/2}[1+|b\rangle c\langle b|V],$$

where $|b\rangle$ is an arbitrary state with variational parameters and c is an arbitrary constant. This leads to a separable F, and we find

$$F=\pm[V+V|b\rangle B\langle b|V]$$

and

$$F^{-1}=\pm[1/V-|b\rangle c^2B(B-c)^{-2}\langle b|],$$

where

$$B=c(2+c\langle b|V|b\rangle).$$

It is now a simple task to construct T. The arbitrary constants should be chosen so as to minimize T, where

$$T=\mathrm{Tr}[VGVG^\dagger]-[B^2c^2/(B-c)^2]\times[|\langle b|VGV|b\rangle|^2-\langle b|V|b\rangle\langle b|VGVG^\dagger V|b\rangle].$$

Schwinger has shown[25] that T gives an upper bound on the number of bound states. Therefore we see that the separable choice for M yields a variational bound for this number.

[21] N. Khuri, Phys. Rev. **107**, 1148 (1957).
[22] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1961).
[23] M. Baker, Ann. Phys. (N. Y.) 4, 271 (1958).
[24] M. Scadron, S. Weinberg, and J. Wright, Phys. Rev. **135**, B202 (1964). See also K. Meetz, J. Math. Phys. **3**, 690 (1962).
[25] J. Schwinger, Proc. Natl. Acad. Sci. (U. S.) **47**, 122 (1961).

If $V(r)$ falls off exponentially with range R, and F is chosen to fall off the same way, then Eq. (7) tells us that T is finite even if (Imk) is continued to negative values. One can therefore continue T to the second energy sheet until $2(\mathrm{Im}k)=-R^{-1}$, which allows us to define the determinant $D(E)$ on the second sheet in this strip. This result will be important later when we construct the partial-wave amplitudes by an analytic continuation of the determinant.

The important point in this discussion is the fact that if F, F^{-1}, and T exist, then D is an entire function of the coupling constant, and does *not* depend on F. Neither does the resolvent K. The F's simply serve as a device for getting a finite bound on the series for D. Having shown that suitable F's exist, we will not explicitly write then down from now on.

The conditions on $V(r)$ which guarantee the existence of T can be easily ascertained if the angular integration in Eq. (7) is carried out and the variable r' is changed to x, where $r'=rx$. The result is that the potential must be smaller than $1/r^2$ at infinity and smaller than $1/r^2$ at the origin. Actually, it is a simple matter to find L and M's which allow D to exist for quite singular potentials, but we shall not make use of this possibility here; it will be important in a later discussion of the Bethe-Salpeter equation.

The essential feature of the examples quoted above is that the product LM is of the form

$$LM=1+v+f(v),$$

where $\mathrm{Tr}f(v)$ exists. Therefore, there are an infinite number of ways of making Fredholm theory work. It is clear that the freedom of choice for $f(v)$ corresponds to the obvious freedom of rearranging the convergent power series expansions of the Fredholm method. In specific calculations it is possible to take advantage of this arbitrariness by using physical insight to make a judicious choice for L and M to simplify the calculation of D (that is, to make D as close to unity as possible).

Let us now turn to scattering in a state of definite angular momentum in order to derive bounds on the phase shift. The partial wave Green's function g_l satisfies Eq. (1) with G_l given, say, in coordinate space by

$$G_l(r,r',k)=-(i/k)U_l(r_<)V_l(r_>), \tag{8}$$

where

$$U_l(r)=krj_l(kr),$$
$$V_l(r)=krh_l^{(1)}(kr),$$

where j_l and $h_l^{(1)}$ are the conventially normalized spherical Bessel functions. For later use, we record here the static or zero-energy Green's function

$$G_l(r,r';0)=[1/(2l+1)]r_<(r_</r_>)^l. \tag{9}$$

For nonzero energy, one finds that $\mathrm{Tr}v_l$, where $v_l\equiv G_lV$, exists if the potential is not larger than $1/r$ at infinity and is no worse than $1/r^2$ at the origin. In this case, both L and M may be taken to be unity.

Examination of the convergent power-series expansion for $D_l(E)=D_l(k^2)$ shows that each term is analytic in the E plane, with a cut along the positive real axis. This arises from the fact that the only energy dependence is in the free Green's functions which have their spectrum lying along the positive real axis.

Our next problem is to relate the Fredholm determinant to the phase shift and to the scattering amplitude. Along the positive real axis, we have

$$G_l(E\pm i\epsilon)=PG_l\mp(i/k)|kl\rangle\langle kl|, \tag{10}$$

where PF_l is the principal value or standing wave Green's function and $|kl\rangle$ is a solution of the free Schrödinger's equation, normalized so that $\langle r|kl\rangle=U_l(r)$. Using the fact that

$$\det[1+|a\rangle\langle a|B]=1+\langle a|B|a\rangle,$$

we find

$$D_l(E\pm i\epsilon)=\det[1-PGV]\times\{1\pm(i/k)\langle kl|V(1-PGV)^{-1}|kl\rangle\}.$$

However, the matrix element in the curly brackets is just the K matrix, so we immediately see that

$$D_l(E\pm i\epsilon)=\det[1-PGV]\{1\mp i\tan\delta_l\}=|D_l|\exp(\mp i\delta_l). \tag{11}$$

Therefore, the phase of the Fredholm determinant is the negative of the phase shift. Finally, we see that the t matrix is given by

$$t_l(E)=[D_l(E+i\epsilon)-D_l(E-i\epsilon)]/2ikD_l(E+i\epsilon). \tag{12}$$

This is a trivial result in the two-particle case but its generalizations to the many-channel case[4] will be extremely useful in our later discussions. In any calculation, one can use Eq. (12) to define a unitary scattering amplitude from an approximate determinant.

Our next aim is to construct approximate D's which will yield bounds on the phase shift. We will make the further requirement that the bounds be variationally correct and improvable. Let us begin by examining the dependence of the phase shift on the potential. That is, we allow the potential to depend on some parameter x and calculate the derivative of the phase shift with respect to x. As $x\to x+dx$, $v\to v+dv$, $D\to D+dD$, the phase shift must change to $\delta+d\delta$. We will drop the subscript l from now on—no ambiguity will arise. It is directly seen that

$$\mathrm{Im}(dD/D)=-|1+dD/D|\sin d\delta=-d\delta$$

and

$$D+dD=\det[1-GV-GdV]=D\det[1-gdV]=D(1-\mathrm{Tr}gdV).$$

Finally, we can derive the continuum version of

Feynman's theorem,[26] namely,

$$\frac{d\delta(x)}{dx}=+\mathrm{Im}\ \mathrm{Tr}\left(g\frac{dV}{dx}\right)=-\frac{1}{k}\langle\psi(x)|\frac{dV}{dx}|\psi(x)\rangle, \quad (13)$$

where $\psi(x)$ is the exact incoming or outgoing wave function from which g can be constructed. Integration of this formula yields

$$\delta(z)-\delta(y)=-\int_y^z\frac{dx}{k}\langle\psi(x)|\frac{dV(x)}{dx}|\psi(x)\rangle. \quad (14)$$

This shows that the phase shift is monotonic in the potential. That is, if $V_1\geq V_0$, then by choosing

$$V(x)=V_0+x(V_1-V_0),$$

we see that

$$\delta(1)-\delta(0)=-\int_0^1\frac{dx}{k}\langle\psi(x)|\,(V_1-V_0)\,|\psi(x)\rangle\leq 0. \quad (15)$$

Thus the larger (more repulsive) the potential, the smaller the phase shift. This is obviously true for local potentials but Eq. (15) states the same is true of nonlocal and/or energy-dependent potentials. We will call a potential difference positive definite if *all* its diagonal matrix elements are positive, and by (15) one sees that the correponding phase-shift difference is negative definite.

The problem of constructing comparison potentials, which bound the potential of interest and which can be solved explicitly, is easily accomplished with the aid of a generalization of Schwartz's inequality. Let the potential V be positive, that is, repulsive (we will relax this requirement later), and consider the form

$$\{\langle\psi|+\sum_i c_i^*\langle i|\}V\{|\psi\rangle+\sum_i c_i|i\rangle\}\geq 0,$$

where $|i\rangle$ is a set of N arbitrary functions. If the expression is minimized with respect to the c_i's, then we find

$$\langle\psi|V|\psi\rangle\geq\sum_{i,j}\langle\psi|V|i\rangle A_{ij}\langle j|V|\psi\rangle,$$

where A_{ij} is the inverse of the matrix $\langle i|V|j\rangle$. Since $|\psi\rangle$ is arbitrary, we can write this in matrix notation as

$$V\geq V|q\rangle A\langle q|V\equiv V_s, \quad (16)$$

where $\langle q|$ and $|q\rangle$ are column and row vectors made up of the set $|i\rangle$. Then the Fredholm determinant for the potential V_s is

$$D^s=\det[1-A\langle q|VGV|q\rangle], \quad (17)$$

and the determinant is taken in the discrete space of the N functions $|i\rangle$. The phase shift is given by

$$\tan\delta^s=-(1/k)\langle u|V|q\rangle \times[\langle q|V-VPGV|q\rangle]^{-1}\langle q|V|u\rangle \quad (18)$$

in matrix notation, and $\delta^s\geq\delta$. If the potential V is negative definite (attractive) then the phase-shift inequality is reversed.

This expression for the phase shift is equivalent to the Schwinger variational principle and the bound property was first proved by Kato[13] under the unnecessary condition that the phase shift be sufficiently small. We see that (18) is a maximum variational principle for $V\leq 0$, and a minimum principle for $V\geq 0$.

It should be noted that as the number of trial functions is increased the bound on the phase shift is always improved. Suppose that a calculation is performed with a set of N trial functions $|i\rangle$. The separable potential is

$$V^N=V|q_N\rangle A^N\langle q_N|V,$$

where $|q_N\rangle$ is an N-dimensional column vector. If one trial function is added, the separable potential becomes

$$V^{N+1}=V|q_{N+1}\rangle A^{N+1}\langle q_{N+1}|V.$$

In order to show that $V^{N+1}\geq V^N$, we introduce the $N+1$-dimensional column vector $|p\rangle$, $|p_i\rangle=|i\rangle$, $i=1,\cdots N$, $|p_{N+1}\rangle=0$, and use Schwartz's inequality with $|p\rangle$. Since

$$V^{N+1}|p\rangle=V|p\rangle$$

and

$$V^{N+1}\geq 0,$$

we have

$$V\geq V^{N+1}\geq\frac{V^{N+1}|p\rangle\langle p|V^{N+1}}{\langle p|V^{N+1}|p\rangle}=V^N.$$

If N is increased until the $|i\rangle$ form a complete set, then the phase shift will converge to the exact value. It is also easily seen that if one trial function in the set $|i\rangle$ is the exact wave function $|\psi\rangle$, then

$$|q\rangle[A^{-1}-\langle q|VPGV|q\rangle]^{-1}\langle q|V|u\rangle=|\psi\rangle, \quad (19)$$

and the phase shift is given correctly by (18).

It is a more difficult matter in practice to obtain the opposite bound. It is necessary to find a solvable potential V_0 such that $V<V_0$. For a positive definite V, one may write

$$V=V_0+(V-V_0)=V_0+V_1,$$
$$V\leq V_t=V_0+V_1|p\rangle B\langle p|V_1,$$

where we have again used the Schwartz inequality and introduced a matrix notation. The matrix B is defined by

$$B^{-1}=\langle p|V_1|p\rangle, \quad (20)$$

where $|p\rangle$ and $\langle p|$ are N component row and column vectors, respectively. The phase shift δ^t is calculated from

$$D=\det[1-G(V_t)]=\det[1-GV_0]\times\det[1-g_0(V_t-V_0)],$$

where $g_0=(1-GV_0)^{-1}G$.

Assuming that g_0 and the corresponding phase shift δ^0 are known, we find for our other bound on the phase

[26] R. P. Feynmann, Phys. Rev. **56**, 340 (1939).

shift

$$\tan(\delta^t-\delta^0)=-(1/k)\langle\psi_0|V_1|p\rangle \times[\langle p|V_1-V_1\,\mathrm{Reg}_0V_1|p\rangle]^{-1}\langle p|V_1|\psi_0\rangle, \quad (21)$$

where ψ_0 is the wave function in the potential V_0 with either incoming or outgoing wave boundary conditions. The real part of g_0 is related to the standing wave Green's function Pg_0 by

$$\mathrm{Reg}_0=Pg_0+|\phi_0\rangle\langle\phi_0|\cos\delta^0\sin\delta^0,$$

where ϕ_0 is the standing wave solution in the potential V_0. Precisely, ϕ_0 at infinity approaches a unit sine term plus a cosine term times $\tan\delta^0$. Rewriting Eq. (21) in terms of the standing wave quantities yields

$$\begin{aligned}&\tan\delta^t-\tan\delta^0\\&=-(1/k)\langle\phi_0|V_1|p\rangle[\langle p|V_1-V_1Pg_0V_1|p\rangle]^{-1}\langle p|V_1|\phi_0\rangle\\&\equiv-(1/k)\langle\phi_0|V_1|p\rangle C_1\langle p|V_1|\phi_0\rangle. \quad (22)\end{aligned}$$

It is clear from (22) that as $V\to V_0$, the bound becomes exact. It is desirable and even essential for accuracy that (22) also be forced to yield the correct phase shift as $V\to 0$. This is easy to accomplish; it is sufficient to include the free wave function $|u\rangle$ in the set $|p\rangle$. Then we find for $V\sim 0$ that

$$|p\rangle C_1\langle p|V_1|\phi_0\rangle\to|u\rangle$$

by the same reasoning that leads to Eq. (19). As $V\to 0$, the exact wave function for the potential V_t is a plane wave and obviously $\tan\delta^t=0$. This does not necessarily mean that δ^t is zero, since it could also be a multiple of π. Now, if $\delta(V)$ differs from δ^0 by more than $N\pi$, then δ^t does not provide an accurate bound. To see this, we note that as V_1 increases from zero, the determinant of C_1^{-1} in Eq. (22) can vanish at most N times. Therefore $(\delta^t-\delta^0)$ cannot be larger in magnitude than $N\pi$. Computationally, this simply means that one should increase the number of trial functions until δ^t stops jumping by π.

Even if V is not small it is advantageous to include a plane wave $|u\rangle$ in the set $|p\rangle$, since then one finds

$$\begin{aligned}&+(1/k)\langle\phi_0|V_1|p\rangle C_1\langle p|V_1|\phi_0\rangle\\&\qquad=\tan\delta^0+\langle u|V+VPg_0V|u\rangle+O(V^2).\end{aligned}$$

Thus the explicit contribution of V_0, namely, δ^0, will cancel. Again, if the exact wave function is among the set $|p\rangle$, then Eq. (22) will yield the correct phase shift.

B. Binding Energies

In our discussion of multichannel and multiparticle scattering, it will be necessary to have both upper and lower bounds on the energy of any bounds states that occur. Let us handle that problem now and we will start by considering a Hamiltonian with a single (this condition will be relaxed later) bound state at $E=E_0<0$ and a continuous spectrum starting at $E=0$. An upper bound on E_0 can be obtained by the Rayleigh-Ritz variational principle. Let us suppose that we have a normalized trial function B that is good enough so that

$$E_0\leq\langle B|H|B\rangle\equiv E_0'<0.$$

In this case a lower bound on E_0 can be obtained by an extension of the method of Bazley and Fox.[11] They show that if a solvable Hamiltonian H_s can be constructed such that $H_s\leq H$, then the eigenvalues of H_s are less than the corresponding eigenvalues of H. This is easy to prove using Feynman's theorem.[26] In order to construct H_s, it is sufficient to write H as the sum of a separable term and a term that is positive definite. The positive definite term can then be made separable by using the Schwartz inequality as was discussed earlier.

Following Rosenberg *et al.*,[27] let us imagine performing a two-dimensional Rayleigh-Ritz calculation on H using $|B\rangle$ and any other normalized trial function $|C\rangle$. We will obtain [28] two approximate eigenvalues $F1$ and $F2$ such that

$$E_0\leq F1\leq E',$$

and

$$0\leq F2.$$

Now

$$\langle C|H|C\rangle\langle B|H|B\rangle-\langle B|H|C\rangle\langle C|H|B\rangle=F1\cdot F2$$

and hence

$$\langle C|H|C\rangle-(\langle C|H|B\rangle\langle B|H|C\rangle/E_0')\geq 0.$$

But since C is arbitrary

$$H'\equiv H-(H|B\rangle\langle B|H/E_0')\geq 0, \quad (23)$$

and

$$H=H'+(H|B\rangle\langle B|H/E_0')\geq H_s,$$

where

$$H_s=\frac{H'|A\rangle\langle A|H'}{\langle A|H'|A\rangle}+\frac{H|B\rangle\langle B|H}{E_0'}.$$

Now the lowest eigenvalue of H_s, E_0'', is less than E_0. It should be noted that we really have a variational principle for E_0 and that if either A or B is the exact ground-state wave function for H then $E_0''=E_0$. In any case, we have

$$E_0''\leq E_0\leq E_0'.$$

In a practical calculation where the number of bound states is not known, it is necessary to perform higher order Rayleigh-Ritz calculations until it is no longer possible to obtain eigenvalues that are negative. Since we have developed a variational upper bound for the number of bound states [see the discussion following Eq. (7)], this tells us the maximum number of Rayleigh-Ritz eigenvalues which may be present.

If there are N negative Rayleigh-Ritz eigenvalues $E_1', E_2'\cdots E_N'$, then it is possible to construct N

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

[28] E. A. Hylleraas and B. Undheim, Z. Physik **76**, 759 (1930). See also J. MacDonald, Phys. Rev. **43**, 830 (1933).

orthonormal trial functions $B_1, B_2, \cdots, B_N$. The positive definite operator H' is then given by

$$H' = H - \sum_{i=1}^{N} \frac{H|B_i\rangle\langle B_i|H}{E_i'},$$

and the generalized Schwartz inequality can now be used to obtain lower bounds on all binding energies. Since H' is positive definite, the eigenvalues of the Hamiltonian

$$H_s \equiv \sum_{i=1}^{N} \frac{H|B_i\rangle\langle B_i|H}{E_i'} \leqslant H$$

will also give variational lower bounds on all of the binding energies.

Let us now consider some examples.

III. EXAMPLES AND APPLICATIONS

Since it is always possible to obtain the exact phase shifts in single-channel scattering by a simple numerical integration of the Schrödinger equation, this section is included only to give a few numerical tests of our method and to derive a few more general results. The bounds on the phase shift will be useful only if it is possible to choose separable potentials which lead to simple analytical expressions. For simplicity we restrict ourselves to calculations of scattering lengths, but we will present one calculation for the phase shift for a range of energies.

The first potential we consider is the old favorite

$$V = -(\lambda/r)e^{-r}. \tag{24}$$

The trial wave function will be chosen to be

$$|q\rangle = (r, r^2),$$

which should be appropriate for s waves. The scattering length A^s is given by ($\delta^s = -kA^s$, $k \to 0$)

$$A(\text{exact}) \leq A^s = +\langle r|V|q\rangle \times [\langle q|V - VPGV|q\rangle]^{-1}\langle q|V|r\rangle. \tag{25}$$

We find

$$\langle r|V|q\rangle = -\lambda(1,2),$$

and the other integrals can be easily carried out with the result that

$$A(\text{exact}) \leq A^s = -\lambda[1 - \tfrac{1}{8}\lambda][1 - \tfrac{5}{8}\lambda + \tfrac{1}{32}\lambda^2]^{-1}.$$

The condition for a zero-energy bound state yields a bound on the coupling constant

$$\lambda(\text{exact}) \leq \lambda = 10 \pm (68)^{1/2} = 1.75,\ 81.25. \tag{26}$$

The exact value for the occurrence of the first bound s state is 1.6798, and for the second bound s state, 6.464.

A rough upper bound on the scattering length can be easily calculated by choosing [see Eq. (22)]

$$V_0 = -C/r^2$$

and

$$V_1 = -\lambda(e^{-r}/r) + C/r^2. \tag{27}$$

The optimum choice for C which makes V_1 as small as possible but still positive is $C = \lambda e^{-1}$. The s-wave phase shift for V_0 is

$$\delta^0 = \tfrac{1}{2}L\pi,$$

where

$$2L+1 = (1-4C)^{1/2}; \tag{28}$$

and we assume that C is less than $\frac{1}{4}$ for the moment. The scattering length is easily calculated from Eq. (22) if we assume a single plane-wave trial function

$$A(\text{exact}) \geq A^t = \langle r|V + Vg_0V|r\rangle,$$

where

$$g_0 = -\frac{r_<}{(2L+1)}\left(\frac{r_<}{r_>}\right)^L.$$

These integrals yield

$$A(\text{exact}) \geq A^t = -\lambda - \tfrac{1}{2}\lambda^2 - 4\lambda^2 \int_0^1 dx \frac{x}{(1+x)^3}\left[\frac{x^L}{(2L+1)} - 1\right]. \tag{29}$$

The first two terms are recognized as first- and second-order perturbation theory. The last term vanishes if $C \to 0 (L \to 0)$, and is of order λ^3 if $C = \lambda e^{-1}$. The scattering length bound A^t is infinite when $(2L+1)$ is zero, and this condition together with Eq. (26) yields bounds on the coupling strength required to produce a bound S state

$$e/4 = 0.68 \leq \lambda(\text{exact}) \leq 10 - (68)^{1/2} = 1.75.$$

These bounds are, of course, very rough since we have done no work. They become better, however, if we consider higher partial waves. Our bounds will be expressed in terms of the largest angular momentum l which has a bound state. In terms of the Regge trajectory, we will derive upper and lower bounds on $\alpha(0)$.

The upper bound is again derived by introducing the potential V_0 as in Eq. (27). For arbitrary l, however, Eq. (28) becomes

$$2L+1 = [(2l+1)^2 - 4C]^{1/2}.$$

The vanishing of the square root is again the condition for a zero-energy bound state and the bound on the exact angular momentum α becomes

$$2\alpha + 1 \leq 2(\lambda/e)^{1/2}. \tag{30}$$

The lower bound will be calculated from Eq. (25) by assuming a trial function of the form

$$q = r^b e^{-cr},$$

with two positive variational parameters b and c. The condition for a bound state is

$$\langle q|V|q\rangle = \langle q|VPgV|q\rangle.$$

Evaluation of the integrals leads to the requirement

that

$$\frac{(2l+1)}{I(l,b)}=4b\lambda\frac{(1+2c)^{2b}}{(1+c)^{2b+1}}, \tag{31}$$

where

$$I(l,b)=\int_0^1 dx\, x^{l+b}(1+x)^{-1-2b}.$$

Since I is a decreasing function of l, the parameter c will be chosen to maximize the right-hand side of Eq. (31). This value turns out to be $c=b-\frac{1}{2}$ if $b\geq\frac{1}{2}$, and $c=0$, if $b\leq\frac{1}{2}$. The exact value of the angular momentum α then must satisfy the inequality

$$(2\alpha+1)/I(\alpha,b)\geq 2\lambda[4b/(2b+1)]^{2b+1}, \tag{32}$$

for $b>\frac{1}{2}$ and $\geq 4\lambda b$ if $0<b<\frac{1}{2}$.

Let us test this inequality by calculating the coupling constant required to produce an s-wave and p-wave bound state at zero energies. Choosing $b=1$, a not unreasonable value which simplifies the integrals, we find for the s wave

$$I(0,1)=\tfrac{1}{8},$$
$$\lambda_0\leq 27/16\leq 1.69,$$

and for the p wave

$$I(1,1)=\ln 2-\tfrac{5}{8},$$
$$\lambda_1\leq 9.28.$$

The exact value of λ_1 for the occurrence of a p-wave bound state is 9.080.

This inequality, Eq. (32), is true for all values of b. However, there are two limits in which the bound can be strengthened by choosing the optimum value of b. If $\lambda\to 0$, we see that α is greater than or equal to minus one-half. From Eq. (30), we also see that α is less than or equal to minus one-half. Therefore, the leading Regge trajectory at zero energy goes to $(-\frac{1}{2})$ as the coupling vanishes.

In the limit of large λ, the optimum choice of b can be determined. If the coupling constant is large, then α is also large, and the integral I approaches the bound

$$I(\alpha,b)\geq(\alpha+b+1)^{-1}2^{-1-2b}.$$

Even for $\alpha=0$, $b=1$, this estimate is only wrong by a factor of 2. Solving (32) for α yields

$$2\alpha+1\geq[4\lambda f(y)+y^2/4]^{1/2}-\tfrac{1}{2}y, \tag{33}$$

where

$$f(y)=(1-1/y)^y \quad \text{for } y\geq 2$$
$$=(y-1)2^{-y} \quad \text{for } 1\leq y\leq 2$$

and

$$y=1+2b.$$

As λ gets large, it is easily seen that the optimum value of b is also large, and $f(y)$ becomes

$$f(y)=\exp[y\ln(1-1/y)]$$
$$=e^{-1}[1-(1/2y)+\cdots].$$

The value of y which optimizes the bound is

$$y^4=\lambda/e.$$

The value α in the limit is bounded by

$$2(\lambda/e)^{1/2}\geq 2\alpha+1\geq 2(\lambda/e)^{1/2}-(\lambda/e)^{1/4}+\cdots. \tag{34}$$

This is quite a general result as far as the dependence of α on the coupling constant is concerned. For the exponential potential

$$V=-\Lambda e^{-r},$$

the bounds become

$$4(\Lambda/e^2)^{1/2}\geq 2\alpha+1\geq 4(\Lambda/e^2)^{1/2}-2(\Lambda/e^2)^{1/4}+\cdots. \tag{35}$$

The dependence on the coupling constants of these inequalities seems to be true for quite general potentials, even the square well, as the reader may easily verify. This dependence of α in the strong coupling limit has been found previously by Tiktopoulos and Treiman.[29]

The bounds on α for the Yukawa case may also be compared with the numerical calculations of Ahmadzadeh, Burke, and Tate.[30] The largest value of λ which they considered was $\lambda=8$, and for that value, α turned out to be 0.9. For this value of the coupling constant, the optimum choice of y in Eq. (33) turns out to be between 2 and 2.5. The resultant inequalities compared with the exact values are

$$3.43\geq 2\alpha+1=2.8\geq 2.0.$$

For the value $\lambda=5$, we find y is again approximately 2, and

$$2.72\geq 2\alpha+1=2.04\geq 1.45.$$

These limits are not bad considering the crudeness of the upper bound and the inaccuracy of the estimate used in the lower bound for $I(\alpha,b)$ when α is small. To estimate this latter error, let us evaluate $I(\alpha,b)$ exactly when $\alpha=\frac{1}{2}$, $b=\frac{1}{2}$. We know from the numerical calculations that λ is slightly less then 5. We find

$$I=\ln 2-\tfrac{1}{2}=0.193,$$

whereas our bound yields

$$I_b=0.125.$$

The values of λ given by these two estimates of the integral I are, respectively,

$$\lambda\leq 1/I=5.23$$

and

$$\lambda\leq 1/I_b=8.0.$$

The accuracy of the first result is obvious.

The lower bound on the s-wave phase shift for an attractive Yukawa potential has been calculated for a range of energies. The strength of the potential was

[29] G. Tiktopoulos and S. B. Treiman, Phys. Rev. **135**, B711 (1964).

[30] A. Ahmadzadeh, P. G. Burke, and C. Tate, Phys. Rev. **131**, 1315 (1963).

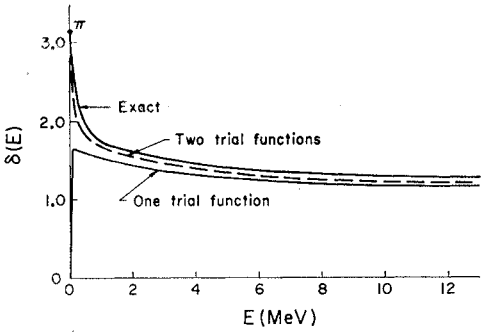

FIG. 1. Comparison of s-wave phase shifts for Yukawa potential with a bound state for nucleon-nucleon scattering. Trial functions were chosen to be of the form $\sin Kr$.

chosen so that there was a bound state very near zero energy, the range was chosen to be one fermi, and the mass corresponds to nucleon-nucleon scattering. The results are presented in Fig. 1 for one and two trial functions and compared with an exact numerical calculation. The trial functions were chosen to be

$$|q_1\rangle=\sin k_1 r, \quad |q_2\rangle=\sin k_2 r.$$

The variational parameters k_1 and k_2 were chosen to (roughly) maximize the phase shift at each energy point calculated. It should be noted that the value of λ which we chose gives a particularly severe test of the theory. If λ was less than 1.69 then there is no bound state and all the phase-shift curves would start out at zero. If λ was greater than 2, then even the one trial function case has a bound state and all the curves would start out at π.

IV. MULTICHANNEL SCATTERING

In this section we will consider the problem of multichannel scattering. We will restrict ourselves to the case in which there are a finite number of channels each of which contains two particles. Our starting point is again the Lippmann-Schwinger equation. However, the operators are now to be considered to be matrices whose rows or columns are labeled by the channels. The potential matrix is symmetric and the free Green's function is a diagonal matrix whose elements are given by

$$G_{ij}=\delta_{ij}G(k_i r)\equiv\delta_{ij}G_i. \tag{36}$$

$G(k_i r)$ is the two-particle free Green's function employed in Sec. II and k_i is the wave number in the ith channel. If the threshold for the ith channel is at energy E_i and the reduced mass in that channel is m_i, then k_i is given by

$$E=\hbar^2 k_i^2/2m_i+E_i, \tag{37}$$

where E is the total energy of the system.

Just as in the case of single-channel scattering, Fredholm theory can not be applied directly to the three-dimensional Lippmann-Schwinger equation. Again the problem is that

$$\mathrm{Tr}[GV]=\sum_i \mathrm{Tr}[G_i V_{ii}] \tag{38}$$

does not exist. However, this defect can again be remedied by the same method that was used in the single-channel problem, namely, by choosing appropriate L and M kernels.

Let us now consider the problem of scattering in a state of definite angular momentum. If there are N channels, it is convenient to define N column vectors $U^l{}_1,\cdots,U^l{}_N$ such that in coordinate space, the ith component of the jth vector $U^l{}_{ij}$ is given by

$$U^l{}_{ij}(r)=\delta_{ij}k_i r j_l(k_i r).$$

In terms of these vectors, the T matrix is given by

$$T_{ij}{}^l=\langle U_i{}^l|\, V\frac{1}{1-G_l V}|\, U_j{}^l\rangle(k_i k_j)^{-1/2},$$

which for the diagonal elements can be written in terms of the phase shift as

$$T_{jj}=-e^{i\delta}\sin\delta.$$

The free Green's function G_l is a diagonal matrix with elements in coordinate space given by

$$G_{l_{ij}}=-(i/k_j)k_j r_< j_l(k_j r_<)k_j r_> h_l{}^{(1)}(k_j r_>). \tag{39}$$

It will often be convenient to write it in the form

$$G_{+l}(E+i\epsilon)=PG_l-i\sum_{j=1}^{N}\frac{1}{k_j}|\, U_j{}^l\rangle\langle U_j{}^l|,$$

where PG_l is a diagonal matrix whose elements are the appropriate standing wave Green's functions.

If the diagonal elements of the potential matrix are smaller than $1/r$ at infinity and smaller then $1/r^2$ at the origin, then $\mathrm{Tr}G_l V$ exists and both L and M may be taken to be unity. By examining the Fredholm expansion for $D_l(E)$, we see that each term is an analytic in the E plane with cuts starting at the threshold of each channel and running along the positive real axis. This is true even if there are anomalous thresholds which explicitly show up in the k plane.[6]

In order to construct the T_l matrix from the Fredholm determinant, we must consider particular "complex conjugate" D's. D_+ is defined to be the value of D on the real axis just above all of the cuts. D_{j-} is obtained by following the path in Fig. 2. The dotted

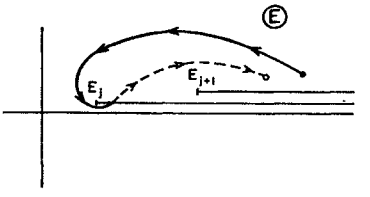

FIG. 2. Continuation path.

part of the path is on the second sheet of the E_j cut. This path takes the complex conjugate of quantities that have branch points at E_j, but leaves other quantities unchanged. As a result, the Green's functions become

$$G_{lj-}=G_{l+}+(2i/k_j)\,|U^l{}_j\rangle\langle U^l{}_j|\,, \tag{40}$$

so that

$$D_{j-}=\det[1-G_{lj-}V]$$
$$=D_+\left[1-\frac{2i}{k_j}\langle U_j{}^l|\,V\frac{1}{1-G_{l+}V}|\,U_j{}^l\rangle\right] \tag{41}$$

and we have

$$T_{jj}=(D_+-D_{j-})/2iD_+. \tag{42}$$

In order to obtain the off-diagonal elements of T, it is necessary to consider D_{k-j-}, which is obtained by going onto the second sheet of both the E_k and E_j cuts. Using the fact that

$$G_{lk-j+}=G_{l+}+(2i/k_k)\,|U^l{}_k\rangle \times\langle U^l{}_k|+(2i/k_j)\,|U^l{}_j\rangle\langle U^l{}_j| \tag{43}$$

and that

$$\det[1+A\,|U_k\rangle\langle U_k|B+A\,|U_j\rangle\langle U_j|B] \begin{vmatrix}1+\langle U_k|BA\,|U_k\rangle & \langle U_k|BA\,|U_j\rangle\\ \langle U_j|BA\,|U_k\rangle & 1+\langle U_j|BA\,|U_i\rangle\end{vmatrix}, \tag{44}$$

we find

$$D_{k-j-}=D_+[(1-2iT_{kk})(1-2iT_{jj})+4T_{kj}T_{jk}]. \tag{45}$$

As a result,[4,6]

$$T_{kj}T_{jk}=T_{kj}{}^2=(D_+D_{k-j-}-D_{k-}D_{j-})/4D_+{}^2. \tag{46}$$

The reader can easily check that the T matrix defined by (42) and (46) satisfies unitarity. In fact, starting from any approximate D that has the same analyticity properties as the exact determinant, Eqs. (42) and (46) can be used to define an approximate but symmetric T matrix that satisfies unitarity exactly.

Our next objective is to obtain approximate D's that will yield bounds on as many of the scattering parameters as possible. We will be concerned with the case in which $E_1<E<E_2$, so that only elastic scattering is possible. It is convenient to write our operators in the matrix form

$$Q=\begin{pmatrix}Q_{11} & Q_{12}\\ Q_{21} & Q_{22}\end{pmatrix}, \tag{47}$$

where Q_{21} is an $N-1$-dimensional column matrix with components Q_{21}, $Q_{31},\cdots,Q_{N1}$, and Q_{12} is an $N-1$-dimensional row matrix. Finally, the operator Q_{22} stands for an $N-1$-dimensional square matrix.

The Fredholm determinant can now be written as

$$D=\det[1-G_{22}V_{22}] \times\det[1-G_{11}V_{11}-G_{11}V_{12}g_{22}V_{21}], \tag{48}$$

where

$$g_{22}=[1/(1-G_{22}V_{22})]G_{22}=1/(E-H_{22}). \tag{49}$$

The angular momentum label l has been omitted. Below the first inelastic threshold G_{22} is real, so that $D_{1-}=(D_{1+})^*$. As a result, T_{11} can be written in the form

$$T_{11}=-e^{i\delta}\sin\delta\,, \tag{50}$$

and $D=|D|e^{-i\delta}$, where δ is real. Since the first determinant in Eq. (48) is real, we have a one-channel problem with an effective real potential W given by

$$W=V_{11}+V_{12}g_{22}V_{21}\,, \tag{51}$$

and we know from the results of Sec. II that one can obtain an upper (lower) bound on δ in the elastic region by replacing W by a smaller (larger) potential. Since it is almost as easy to integrate the one-channel Schrödinger equation numerically as to apply the bounds discussed in the previous section, the real problem here is to find a bound for g_{22} and hence W.

A. No Bound States in the Inelastic Channels

If H_{22} does not have any bound states, then g_{22} is a negative definite operator for $E<E_2$. Schwartz's inequality then gives

$$g_{22}\leq g_{22}|s\rangle\frac{1}{\langle s|g_{22}|s\rangle}\langle s|g_{22}\,, \tag{52}$$

where $|s\rangle$ is an arbitrary $N-1$-dimensional column vector. We obtain a more useful form by taking $|s\rangle=(E-H_{22})|q\rangle$ so that

$$g_{22}\leq|q\rangle\frac{1}{\langle q|E-H_{22}|q\rangle}\langle q|\,. \tag{53}$$

Using this result and Eq. (51), we find

$$W\leq W_L\equiv V_{11}+V_{12}|q\rangle\frac{1}{\langle q|(E-H_{22})|q\rangle}\langle q|V_{21}. \tag{54}$$

Writing W_L out explicitly in configuration space, we have

$$W_L(r,r')=V_{11}(r)\delta(r-r') +\sum_{i,j=2}^{N}\frac{V_{1i}(r)q_i(r)q_j(r')V_{j1}(r')}{\langle q|E-H_{22}|q\rangle}, \tag{55}$$

where $q_i(r)$ is the ith component of the column vector $|q\rangle$. (We have chosen its indices to run from 2 to N.) If the one-channel Schrödinger equation is solved with the potential W_L, then the resulting phase shift δ_L is a lower bound on the true δ. If the exact wave function for the N-channel problem is $\psi=(\psi_1\psi_2)$, and if $\langle q|$ is chosen to be ψ_2, then it is easy to see from the Schrödinger equation that $\delta_L=\delta$. In addition, if $\langle q=\psi_2+\delta\psi_2$ then $\delta-\delta_L$ is of order $(\delta\psi)^2$ if $\delta\psi$ is small. We thus have a variational principle for the phase shift that gives the exact answer if the trial function is exact and gives a lower bound no matter how bad the trial function is. The bound can of course be improved indefinitely by

using more and more complicated trial functions. It can also be improved by using the generalized Schwartz inequality discussed in Sec. II. If $|q_1\rangle$, $|q_2\rangle\cdots|q_M\rangle$ are a set of arbitrary trial column vectors, then

$$g_{22}\leq\sum_{i,j=1}^{M}|q_i\rangle A_{ij}\langle q_j|\leq\frac{|q_1\rangle\langle q_1|}{\langle q_1|E-H_{22}|q_1\rangle}, \tag{56}$$

where A_{ij} is the inverse of the matrix $\langle q_i|E-H_{22}|q_j\rangle$. As a result,

$$W\leq W_L{}^{(M)}\equiv V_{11}+\sum_{i,j=1}^{M}V_{12}|q_i\rangle A_{ij}\langle q_j|V_{21},$$

and

$$W_L{}^{(M)}\leq W_L{}^{(1)}\equiv V_{11}+\frac{V_{12}|q_1\rangle\langle q_1|V_{21}}{\langle q_1|(E-H_{22})|q_1\rangle}. \tag{57}$$

Also we have

$$\delta\geq\delta_L{}^{(M)}\geq\delta_L{}^{(1)}.$$

Again, if ψ_2 is included in the set q_i then $\delta_L{}^{(M)}=\delta$.

In order to obtain an upper bound on the phase shift, it is necessary to construct an operator that is smaller (more negative) than g_{22}. Now

$$g_{22}(E)=[(E-E_2)-(H_{22}-E_2)]^{-1},$$

and if H_{22} has no bound states, and E_2 is the lowest inelastic threshold, then $H_{22}-E_2\geq 0$. Since $E_2-E\geq 0$, g_{22} will decrease if we replace $(H_{22}-E_2)$ by a smaller operator. To make this precise we first note that

$$(H_{22}-E_2)\geq(H_{22}-E_2)|p\rangle\frac{1}{\langle p|H_{22}-E_2|p\rangle}\langle p|(H_{22}-E_2)$$
$$\equiv(H_{22}-E_2)_s, \tag{58}$$

where p is an arbitrary $N-1$-dimensional column vector. Now consider the Green's function

$$g_{22}(x)=[(E-E_2)-(H_{22}-E_2)$$
$$-x((H_{22}-E_2)_s-(H_{22}-E_2))]^{-1}, \tag{59}$$

where

$$g_{22}(0)=g_{22}$$

and

$$g_{22}(1)=[(E-E_2)-(H_{22}-E_2)_s]^{-1}$$
$$=(E-E_2)^{-1}\{1+F|p\rangle[\langle p|F(1-F)|p\rangle]^{-1}\langle p|F\}, \tag{60}$$

where $F=(H_{22}-E_2)(E-E_2)^{-1}$. In order to show that $g_{22}(1)\leq g_{22}(0)$, it is necessary to show that for any state $\langle f|$,

$$\langle f|g_{22}(1)-g_{22}(0)|f\rangle\leq 0. \tag{61}$$

Noting the identity

$$J\equiv\langle f|g_{22}|f\rangle-\langle f|g_{22}(0)|f\rangle=\int_0^1 dx\frac{d}{dx}\langle f|g_{22}(x)|f\rangle$$
$$=\int_0^1 dx\langle f|g_{22}(x)[(H_{22}-E_2)_s-(H_{22}-E_2)]g_{22}(x)|f\rangle,$$

it follows from Schwartz's inequality that

$$J\leq 0. \tag{62}$$

Finally, we see that

$$W\geq W_u\equiv V_{11}+V_{12}g_{22}(1)V_{21}. \tag{63}$$

If the one-channel Schrödinger equation is solved with the potential W_u, the resulting phase shift δ_u will be an upper bound on δ. Again if $p=\psi_2$, then $\delta_u=\delta$, and if $p=\psi_2+\delta\psi$, then $\delta_u-\delta$ is of order $\delta\psi^2$ for small $\delta\psi$. We thus have a variational principle that gives the exact phase shift if the trial function is exact and gives an upper bound on the phase shift for any other trial function. Again the bound can be improved by using the generalized Schwartz inequality

$$(H_{22}-E_2)\geq\sum_{i,j=1}^{M}(H_{22}-E_2)|p_i\rangle B_{ij}\langle p_j|(H_{22}-E_2)$$
$$\equiv(H_{22}-E_2)_s{}^M.$$

It is easy to see that

$$(H_{22}-E_2)_s{}^M\geq(H_{22}-E_2)_s{}^1.$$

B_{ij} is the inverse of the matrix $\langle p_i|H_{22}-E_2|p_j\rangle$ and $p_1\cdots p^M$ is a set of M arbitrary trial functions. As a result,

$$g_{22}\geq g^M{}_{22}(1)=[(E-E_2)-(H_{22}-E_2)^M{}_s]^{-1}$$
$$\geq g^1{}_{22}(1) \tag{64}$$

and the corresponding inequalities on the phase shifts are obvious from our previous discussion.

At this juncture it should be noted that there is an alternative procedure which may yield a more accurate bound than Eq. (64) (which involves matrix elements of the square of the Hamiltonian). This is the method of Bazley and Fox[11] who require that H be the sum of a solvable Hamiltonian and a positive definite potential. Then if the positive definite part is made separable, a lower bound on the Green's function can be constructed. This method can be carried through only in special cases, however.

B. Bound States in the Inelastic Channels

Up to now it has been assumed that H_{22} does not have any bound states, but this restriction can easily be removed. Our minimum principle is actually valid even if H_{22} does have bound states.[31] However, in order to obtain a maximum principle, it is necessary to consider the bound-state problem in detail. It is probably also necessary to do so in order to obtain accurate lower bounds. Let us first consider the case in which there is a single bound state at energy E_0. The first problem is to obtain an upper bound, E_0', and a lower bound, E_0'', on the binding energy. This problem has already been discussed in Sec. II.B. For $E<E_0''$ there is no change

[31] R. Sugar, Ph.D. thesis, Princeton University (unpublished). See also the last part of Sec. C.

in the calculation of the lower bound on the phase shift. The upper bound calculation also goes through if E_2 is replaced by E_0'' everywhere that it occurs in Eqs. (58)–(65). For $E \geq E_0'$, g_{22} has a discreet eigenvalue, $(E-E_0)^{-1}>0$, and a continuum of negative eigenvalues running from 0 to $(E-E_2)^{-1}$. In order to obtain bounds on g_{22}, it is desirable to separate off a part that is negative definite. The procedure is the same as in II.B. Let b be the normalized trial function that yields the upper bound energy E_0',

$$E_0 \leq \langle b|H_{22}|b\rangle \equiv E_0' < 0.$$

We now imagine performing a two-dimensional Rayleigh-Ritz calculation for bounds on the two largest eigenvalues of $(-g_{22})$. If one of the trial functions is chosen to be $|f\rangle=(E-H_{22})|b\rangle$, then the method of II.B, see Eq. (23), yields

$$g'_{22} \equiv g_{22} - |b\rangle(E-E_0')^{-1}\langle b| \leq 0.$$

Defining the projection operator $P=1-|f\rangle\langle f|f\rangle^{-1}\langle f|$, it is easy to see that

$$g'_{22}=P[P(E-H_{22})P]^{-1}P.$$

Since g'_{22} is negative definite for $E_0'<E<E_2$, it is possible to obtain a lower bound on the phase shift in this energy region by making g'_{22} separable.

In order to obtain an upper bound on the phase shift, we note that if H_{22} has no bound states between E_0 and E_2, then the quantity J, defined by

$$E-H_{22}=E-E_2-J,$$

has one negative eigenvalue and a positive spectrum. As before [see Eq. (23)] we may write

$$J=J'+J|b\rangle(E_0'-E_2)^{-1}\langle b|J=J'+J_s$$

and J' is a positive definite operator. This allows the Schwartz inequality to be applied, and our previous arguments [see Eq. (62)] lead to

$$g_{22} \geq [E-E_2-J_s-J'_s]^{-1},$$

which immediately yields an upper bound potential.

It should be noted that we still have variational principles for both bounds. If the trial function that makes g'_{22} separable is chosen to be ψ_2, then both the upper and lower bound phase shifts will be exact even if the trial wave function for the bound state is not exact.

The generalization to the case of N bound states is obvious. Let $b_1, b_2, \cdots, b_N$ be the orthonormal Rayleigh-Ritz eigenfunctions that give the upper bound energies $E_1', E_2', \cdots, E_N'$. Then for $E_i' \leq E \leq E_{i+1}''$, where E_{i+1}'' is the lower bound on the energy of the $(i+1)$ bound state, we have

$$g_{22}' \equiv g_{22} - \sum_{j=1}^{i} \frac{|b_j\rangle\langle b_j|}{E-E_j'} \leq 0$$

and

$$J'=J-\sum_{j=1}^{i} J|b_j\rangle(E-E_j')^{-1}\langle b_j|J \geqslant 0,$$

where

$$J=H_{22}-E_{i+1}''.$$

Both the upper and lower bound calculations now go through as before.

C. Extensions Above the Inelastic Threshold

It is possible to extend the previous results to energies above the inelastic threshold. We will consider only two open two-particle channels, but the extension to any number of open channels is straightforward.[31] The potential matrix will be written in the form

$$\begin{pmatrix} V & V_N \\ V_N & V_{NN} \end{pmatrix},$$

where V, V_N, and V_{NN} are 2×2, $2\times N$, and $N\times N$ dimensional matrices, respectively. N is the number of closed channels. The effective potential is

$$W=V+V_N[E-H_{NN}]^{-1}V_N=V+V_N g_N V_N.$$

Standing wave boundary conditions will be used for the free Green's function in the open channels G. Both G and W are of course two-dimensional matrices. The K matrix is given by

$$K_{ij}=-\langle u_i|W[1-GW]^{-1}|u_j\rangle(k_i k_j)^{-1/2},$$

or in matrix notation

$$K=-k^{-1/2}W[1-GW]^{-1}k^{-1/2}.$$

If W depends on a parameter x, then

$$dK(x)/d(x)=-k^{-1/2}[1-WG]^{-1}[dW(x)/dx] \times[1-GW(x)]^{-1}k^{-1/2}. \quad (65)$$

Taking the expectation value of both sides of (65) in an arbitrary state ψ and integrating from 0 to 1, we find

$$\langle\psi|K(1)-K(0)|\psi\rangle=-\int_0^1 dx\langle\phi(x)|\frac{dW(x)}{dx}|\phi(x)\rangle, \quad (66)$$

where $|\phi(x)\rangle=[1-GW(x)]^{-1}k^{-1/2}|\psi\rangle$.

Using the methods of Sec. IV [see Eqs. (52)–(63)], it is possible to construct upper and lower bound potentials, W_u and W_l, such that for any state, ϕ,

$$\langle\phi|W_l|\phi\rangle \geqslant \langle\phi|W|\phi\rangle \geqslant \langle\phi|W_u|\phi\rangle.$$

The derivation of these inequalities is based on the Schwartz inequality and therefore is not affected by the fact that ϕ is now a two-dimensional column vector. Substituting the potentials

$$W_{u,l}(x) \equiv W_{u,l}+x(W-W_{u,l}) \quad (67)$$

into Eq. (66), we find

$$\langle\psi|K^u|\psi\rangle\geqslant\langle\psi|K|\psi\rangle\geqslant\langle\psi|K^l|\psi\rangle,$$

where K^u and K^l are the K matrices for the potentials W_u and W_l. These inequalities are to be understood in terms of the corresponding phase shifts, $K_{ij}=\tan\delta_{ij}$. That is, one must keep track of the branches of the tangent.

If we choose a ψ which has only one open channel component, $\psi=u_i$, $i=1$, 2, then we find

$$K^u{}_{ii}\geqslant K_{ii}\geqslant K^l{}_{ii}.$$

If we define

$$k\equiv K_{11}+K_{22}+2K_{12},$$

then taking $\psi=u_1+u_2$ gives

$$k^u\geqslant k\geqslant k^l.$$

As a result

$$K^u{}_{12}+\Delta\geqslant K_{12}\geqslant K^l{}_{12}-\Delta,$$

where

$$\Delta\equiv\tfrac{1}{2}\,\mathrm{Tr}(K^u-K^l).$$

We therefore have derived variational upper and lower bounds on all elements of the K matrix. In turn, such relations lead to upper and lower bounds on the cross sections for both elastic and inelastic processes.

Equation (67) represents only one method of embedding W in a one-parameter family of potentials. It is sometimes convenient to proceed in a more general fashion. For example, it was mentioned that our lower bound variational principle really does not need to be modified when H_{NN} has bound states. To prove this it is sufficient to construct a potential $W(x)$ such that

$$W(1)=W,$$
$$W(0)=W_l=V_N|q\rangle\langle q|E-H_{NN}|q\rangle^{-1}\langle q|V_N+V,$$
$$dW(x)/dx\leqslant 0,\quad 0\leqslant x\leqslant 1,$$

even if H_{NN} has bound states. We write $W(x)$ in the form

$$W(x)=W(0)+xV_NB(x)^{-1}V_N,$$

then the derivative becomes

$$\frac{dW(x)}{dx}=V_NB(x)^{-1}\left[B(x)-x\frac{dB(x)}{dx}\right]B(x)^{-1}V_N.$$

If we choose

$$B(x)=E-T_{NN}-xV_{NN}+\frac{x}{1-x}|Q\rangle\langle Q|$$
$$=g(x)^{-1}+\frac{x}{1-x}|Q\rangle\langle Q|,$$

where T_{NN} is the kinetic energy operator in the closed channels, and $|Q\rangle$ will be chosen later, then we find

$$B-x\frac{dB}{dx}=E-T_{NN}-\frac{x^2}{(1-x)^2}|Q\rangle\langle Q|.$$

As a result, dW/dx is negative definite for E below the first threshold of T_{NN}. Now

$$B(x)^{-1}=g(x)-g(x)|Q\rangle\left[\frac{1-x}{x}+\langle Q|g(x)|Q\rangle\right]^{-1}\langle Q|g(x),$$

so that the choice

$$|Q\rangle=Cg(1)^{-1}|q\rangle$$

leads to

$$W(1)=W,$$
$$W(0)=W_l,$$

and our result follows at once.

V. THREE-PARTICLE SYSTEMS

The most difficult part of the three-particle problem, besides actually solving it, is to develop a concise notation for all the different functions that must be introduced. The Hamiltonian for three particles with labels 1, 2, and 3 will be written as

$$H=T+V=T+V_1+V_2+V_3,$$

where T is the sum of the kinetic energy operators. The V_i are the pairwise potentials, and i labels the particle which is not interacting, that is, $V_1=V_1(r_{23})$. An intrinsic three-particle interaction can be added without difficulty if it vanishes when any one particle is removed to infinity. If the three-particle potential does not vanish, one can be introduced which does by subtracting the three pairwise potentials which remain as each particle is removed and adding them back into the V_i. In the following discussion we will assume for simplicity that all three particles are distinguishable. If two of the particles are identical, then one should imagine that all of the following effective K-matrix operators are placed between projection operators which guarantee the symmetry or antisymmetry of the states involved.[31]

In order to discuss the total problem with Hamiltonian H, three subsidiary and simpler problems are introduced with Hamiltonians

$$H_i=T+V_i,$$

and Green's functions which satisfy

$$g_i=G+GV_ig_i=G+v_ig_i,$$

where G is the three-particle free Green's function which depends on the total energy E. Since the Green's functions g_i involve one free and two interacting particles, they can be solved by the methods described in Sec. II. Therefore, we are guaranteed that the resolvents

$$K_i=(1-v_i)^{-1},$$

exist and can be constructed. Also, the associated T matrices, which are defined by

$$T_i=V_iK_i,$$

exist, and can be constructed by the Fredholm method.

It should be stressed that these resolvants are Fredholm in the two-particle space of variables but *not* Fredholm in the three-particle space. It is this fact which will allow us to show that a Fredholm solution exists for the complete three-particle problem.

The total Green's function satisfies the equation

$$g=G+GVg\equiv G+vg.$$

As before, we will write the solution in the form

$$g=L[M(1-v)L]^{-1}MG. \tag{68}$$

This will make sense only if M^{-1} and the determinant D exists, where

$$D\equiv\det[M(1-v)L]. \tag{69}$$

If one tries to choose $M=L=1$, then D will exist if

$$\mathrm{Tr}v^N=\mathrm{Tr}v_i^N+\cdots$$

exists for $N=1, 2, \cdots$. Since the trace involves an integration over the coordinates of the ith particles, which is not localized by the potential v_i, this integral is infinite for all values of N. These troublesome terms arise from the disconnected graphs and must be eliminated from D if it is to exist. This is easily accomplished by choosing L and M so that the determinant involves at least two different v_i's in each term. These terms give rise to graphs with a connected structure and D will at least have the possibility of existing.

Again, as in the single-channel case, there are an infinite number of L and M's which give rise to a connected and finite determinant. With

$$M=1$$

and

$$L=(1+C)[K_1+K_2+K_3-2],$$

where C is a connected operator, we find

$$\begin{aligned}L(1-v)M&=(1+C)[1-v_1K_1(v_2+v_3)\\&\quad-v_2K_2(v_1+v_3)-v_3K_3(v_1+v_2)]\\&\equiv(1+C)[1-C_0].\end{aligned} \tag{70}$$

It is self-evident that this is a connected operator. With $C=0$, it is the same operator as used by Weinberg.[9] The trace of C_0 does not in general exist for a local potential, therefore, if one chooses $C=C_0$, the determinant will then involve the trace of C_0^2 to lowest order. Since this will involve four potentials, it will exist if the pairwise potentials behave decently at the origin and at infinity.[9] This is only one particular choice for L and M, and it should be emphasized that there is no unique way of proceeding.

There are other choices for L and M which have useful properties as we shall see later. We can choose

$$L=1+C,$$
$$M=K_1K_2K_3,$$

then

$$M(1-v)L=[1-K_3v_2K_2v_3-K_3K_2v_1K_1(v_2+v_3)][1+C].$$

This is a connected operator; however, it is not symmetric in the particle labels. This is easily remedied by choosing M to be one-sixth the sum of the permutations of K_1, K_2, and K_3.

Another choice which is convenient in any discussion involving an initially bound state, between particles 2 and 3 say, is

$$L=[K_2+K_3-1][1+C],$$
$$M=K_1,$$

which leads to the connected operator

$$\begin{aligned}&M(1-v)L\\&\quad=[1-v_3K_2v_2-v_2K_3v_3-v_1K_1(v_2+v_3)L][1+C].\end{aligned}$$

The point here is that the non-Fredholm part of v is exactly canceled by the non-Fredholm parts of L and M. The question as to which of the infinite choices for L and M is the superior one depends on the details of the potential, and therefore cannot be generally settled.

If one wants to discuss scattering in which the initial state contains a bound state of two particles, say particles 2 and 3, then the choices open for L and M are slightly restricted. The relevant T matrix is defined by

$$g=g_1+g_iT_{i1}g_1, \tag{71}$$

where $i=1, \cdots, 4$, and $g_4\equiv G$. For elastic scattering or a rearrangement collision, $i=1, 2, 3$, and for breakup, $i=4$. In order to ensure that g has a factor of g_1 on the right, we choose $M=K_1$, and then we find

$$T_{i1}=+(V-V_i)L[K_1(1-v)L]^{-1}, \tag{72}$$

where $V_4\equiv 0$. This operator will exist if L is chosen appropriately. As before, there are an infinite number of choices of L which will ensure the existence of the determinant

$$D=\det[K_1(1-v)L], \tag{73}$$

and we will not have to make a specific choice.

Since we will be ultimately interested in getting bounds on the scattering phase shift, some sort of partial-wave decomposition must be made. We will assume that K_1 has the lowest threshold, so that there is an elastic region, and that K_1 has been expanded in partial waves. It is not necessary, but the simplest and most natural choice of a partial-wave basis for the purpose at hand is to couple particles 2 and 3 together and then to couple particle 1 to form a total J. The T-matrix element for this situation is

$$\begin{aligned}T_{11}^J=&-(1/k_1)\langle B,1|(V_2+V_3)L^J\\&\times[K_1^J(1-v^J)L^J]^{-1}|1,B\rangle,\end{aligned} \tag{74}$$

where $|1,B\rangle$ is a direct product of a plane wave for particle 1 and the bound-state wave function of 2 and 3. The Fredholm determinant of interest is

$$D^J=\det[K_1^J(1-v^J)L^J]. \tag{75}$$

It is possible to choose L^J so that it only involves K_2^J

and $K_3{}^J$ since these are the only disconnected graphs left. Therefore L^J is real in the elastic region. From the form of $T_{11}{}^J$, it is clear that the phase shift is the negative of the phase of D^J, just as in the multichannel case.

In order to get bounds on this phase shift, the phase of the determinant must be studied, and to that end it will prove convenient to rewrite D^J so that it takes the same form as in the multichannel case studied in Sec. IV. To that end, let us extract from $g_1{}^J$ the part that contains the lowest bound state wave function of 2 and 3 and call it $|B\rangle$. We will do this by introducing projection operators in the 2–3 coordinates,[12,16]

$$B=|B\rangle\langle B|\,, \qquad R=1-B. \tag{76}$$

This means that

$$g_1{}^J B=Bg_1{}^J=|B\rangle G_1{}^J\langle B|\,,$$

where $G_1{}^J$ is a free-particle outgoing wave Green's function describing the relative motion of particle 1 and the center of mass of the bound state B. This means that $g_1{}^J R$ is real in the elastic region, and has a branch cut starting at the inelastic threshold E_2.

If the determinant is written as (J labels will be omitted from now on)

$$D=\det[(1-g_1(B+R)U(B+R))L],$$

where $U=V_2+V_3$, then it may be separated in a form highly reminiscent of our previous discussion of the multichannel problem;

$$D=D_B D_R D_{BR}, \tag{77}$$

where

$$\begin{aligned}
D_B&=\det[1-g_1BUB],\\
D_R&=\det[(1-g_1RUR)L],\\
D_{BR}&=\det[1-g_1RUB-(1-g_1BUB)^{-1}g_1BURL\\
&\qquad\times\{(1-g_1RUR)L\}^{-1}],\\
&=\det[1-(1-g_1BUB)^{-1}g_1BURL\\
&\qquad\times\{(1-g_1RUR)L\}^{-1}g_1BUB],
\end{aligned}$$

because $RB=0$. Since $R=1-B$, it is directly seen that D_R is a connected determinant since BU is a connected operator. Also, D_R is real in the elastic region, therefore the elastic phase shift comes from the determinant

$$D_e\equiv D_B D_{BR}=\det[1-g_1BWB],$$

where

$$W=U+URL[(1-g_1RUR)L]^{-1}g_1RU.$$

Since B is a projection operator in the relative coordinates of particles 2 and 3, D_e can be reduced to an effective one-particle determinant in the space of the relative coordinate of particle 1 and the bound state. That is,

$$D_e=\det_1[1-G_1\langle B|W|B\rangle], \tag{79}$$

where $\langle B|W|B\rangle$ is the effective potential acting in this one-particle system. If two of the particles are identical, one must inclose W between projection operators which guarantee the correct symmetry and ensure that the inverse operator in the second term of Eq. (78) is taken in the space of such functions.

Our next step is to find upper and lower improvable bounds on this effective potential, since we are assured from the previous discussion that these will lead to bounds on the phase shift in the elastic region. The only formal difference between the three-particle case and the multichannel case discussed earlier is the presence of the operator L which is necessary to yield connected kernels. Our object is to show that it doesn't make any difference in the final formulas. We want to derive upper and lower bounds on the Green's function

$$\begin{aligned}
g_R&=RL[(1-G_1RUR)L]^{-1}G_1R,\\
&=RL[R(E+i\epsilon-H)RL]^{-1}R.
\end{aligned} \tag{80}$$

This Green's function can be written in spectral form by introducing outgoing wave eigenstates $|N\rangle$ of the Hamiltonian RHR:

$$g_R=\sum_N R|N\rangle(E-E_N+i\epsilon)^{-1}\langle N|R. \tag{81}$$

We are assured that a complete enough set of states for RHR exist because it can be written as a sum of H and a separable operator. Therefore one can construct the set using the eigenstates of H which we have demonstrated to be a Fredholm-type operator. The projection operator R will kill any contribution to the sum from the state B. Therefore, the continuous spectrum of E_N starts at E_2. It is now clear that g_R is a negative definite operator in the elastic region *if* RHR does not have any point eigenvalues below E_2. If it does, then we would proceed as in the multichannel case. In any case, if E is below the lowest point in the spectrum of RHR, we have

$$g_R\leq g_R|s\rangle\langle s|g_R|s\rangle^{-1}\langle s|g_R\,,$$

and introducing $|s\rangle=(E-H)R|q\rangle$, the bound becomes

$$g_R\leq R|q\rangle\langle q|R(E-H)R|q\rangle^{-1}\langle q|R. \tag{82}$$

This yields an upper limit on the effective potential which yields, in turn, a *lower* limit on the phase shift:

$$\begin{aligned}
W_l&=\langle B|U|B\rangle\\
&\quad+\langle B|UR|q\rangle\langle q|R(E-H)R|q\rangle^{-1}\langle q|RU|B\rangle.
\end{aligned} \tag{83}$$

This bound is, of course, still true if $\langle q|$ is a column vector made up of trial functions. It is also evidently true that if the set $\langle q|$ contains the exact wave function for the Hamiltonian RHR, W_L will yield the exact phase shift.

The potential W_u which yields an *upper* limit on the phase shift is easily constructed by writing

$$\begin{aligned}
R(E-H)R\leq R(E-E_2)R-R(H-E_2)R|p\rangle\\
\times\langle p|R(H-E_2)R|p\rangle^{-1}\langle p|R(H-E_2)R\,,
\end{aligned}$$

where E_2 is below the lowest value in the spectrum of

RHR. The effective potential is easily evaluated by inverting this separable operator:

$$W_u=\langle B|U|B\rangle+[\langle B|URU|B\rangle/(E-E_2)] +\langle B|Uh|p\rangle A\langle p|hU|B\rangle, \quad (84)$$

where

$$A^{-1}\equiv(E-E_2)\langle p|(E-E_2)h-h^2|p\rangle$$

and

$$h=R(H-E_2)E.$$

Since the last term in Eq. (84) involving the trial functions is positive definite, we can get a crude bound on the phase shift by neglecting it completely and calculating with the first two terms in W_u.

The physics of the problem has now been reduced to making reasonable choices for the trial (vector) functions $|p\rangle$ and $|q\rangle$. If there are nearly overlapping resonances, or cuts on the second sheet,[32] then the choice is clear. For example, in positron-hydrogen scattering, one may want to choose one element of the vector to represent positronium and a free proton and another to contain excited and continuum states of the hydrogen atom and a free positron. One does *not* have to choose the weights associated with these states, since our variational formulas for the effective potentials are independent of the normalization of the components of the vectors $|p\rangle$ and $|q\rangle$.

These bounds will be applied to electron-hydrogen scattering in a later section. However, before leaving the general discussion, it is amusing to note the effect of a discreet eigenvalue of *RHR* in the elastic region. From Eq. (81), the contribution to g_R from such an eigenstate $|r\rangle$ with energy E_r would be

$$g_R\cong R|r\rangle(E-E_r)^{-1}\langle r|R. \quad (85)$$

The potential then has a simple pole in the energy of the form

$$W=W_1+UR|r\rangle(E-E_r)^{-1}\langle r|RU,$$

where W_1 is regular in the neighborhood of E_r. The resulting phase shift is of the form

$$\tan\delta(W)-\tan\delta(W_1)=\langle\phi|UR|r\rangle^2[E-\bar{E}]^{-1}, \quad (86)$$

where

$$\bar{E}=E_r+\langle r|RUg(W_1)UR|r\rangle.$$

The state ϕ is a standing wave solution in the potential W_1, and $g(W_1)$ is the associated standing wave Green's function. We see that there is a resonance associated with this bound state and inevitable level shift.

We have made a rough Rayleigh-Ritz calculation for the ground state of *RHR* for electron-hydrogen scattering. There is at least one bound state in the elastic region slightly below the first inelastic threshold. The resonance associated with this state seems to be showing up in the calculations of Burke and Schey[17] and Temkin.[15] We have not carried this calculation far enough to make this connection precise, nor to remove the apparent discrepancies between the results of these calculations.

Suffice it to say, the preceding discussion can be carried through in the N-particle case. One only has to choose L and M to contain the disconnected graphs in such a way as to cancel the non-Fredholm parts of $(1-v)$. The construction of bounds on the potentials proceeds just as before. For details, the reader is referred to Ref. 31.

VI. ELECTRON-HYDROGEN SCATTERING

As an example of the three-body problem, we will consider the scattering of electrons and positrons by hydrogen atoms. For simplicity, exchange effects will be neglected in the case of electron-hydrogen scattering. It should be emphasized that these effects can be included in our variational principles. The only difference would be that one would have to ask the computer to solve an integro-differential equation, rather than a differential equation. We will work in atomic units so the Hamiltonian is

$$H=-\nabla_x^2-\nabla_y^2-\frac{2}{y}\pm\left(\frac{2}{|\mathbf{x}-\mathbf{y}|}-\frac{2}{x}\right), \quad (87)$$

where the coordinates of the incident particle are denoted by $\mathbf{x}$ and those of the bound electron by $\mathbf{y}$. The upper sign is for electron scattering and the lower sign for positron scattering. In these units the ground-state wave function of the hydrogen atom is

$$|B\rangle=\pi^{-1/2}e^{-y}. \quad (88)$$

The potential seen by the incident particle is

$$U=\pm\left(\frac{2}{|\mathbf{x}-\mathbf{y}|}-\frac{2}{x}\right),$$

and we find

$$V_l(x)=\langle B|U|B\rangle=\mp(2+2/x)e^{-2x}. \quad (89)$$

The potential V_l will of course give a crude lower bound on the phase shift because all the attractive polarization effects have been omitted. A crude upper bound can be obtained from the potential

$$V_u(E,x)\equiv\langle B|U|B\rangle+\frac{\langle B|URU|B\rangle}{E-E_2-1}, \quad (90)$$

where

$$\langle B|URU|B\rangle=-4/x^2+(8/x)(1+1/x)e^{-2x} -4(1+2/x+1/x^2)e^{-4x} +8x\int_0^\infty dt\, e^{-2xt}\ln\left|\frac{1+t}{1-t}\right|. \quad (91)$$

E is the kinetic energy of the incident particle. E_2

[32] R. Blankenbecler, M. L. Goldberger, S. MacDowell, and S. B. Treiman, Phys. Rev. **123**, 692 (1961).

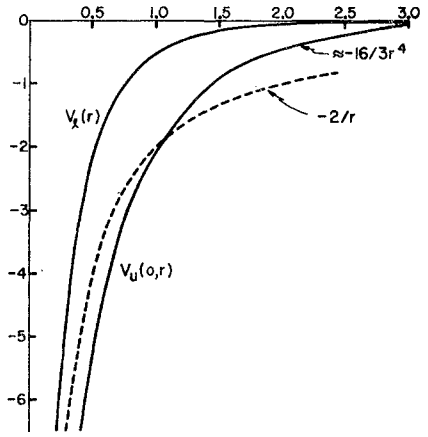

FIG. 3. Upper and lower bound potentials for electron-hydrogen scattering at zero energy. For comparison, the Coulomb potential due to the proton is drawn as the dashed curve.

$=-0.25$ for electron-hydrogen scattering and -0.5 for positron-hydrogen scattering. The potentials $V_u(0,x)$ and $V_l(x)$ are shown in Fig. 3.

The only real physics problem left is the choice of trial functions. In order to perform an accurate calculation it is probably necessary to take into account both the polarization of the hydrogen atom and, in the case of positron-hydrogen scattering, the virtual formation of positronium. As has been pointed out above, each of these effects can be taken into account by a different trial function. The formalism will automatically determine the optimum relative weights of the various trial functions.

A. Polarization Effects

Let us first consider the polarization effects. The average potential seen by the incident particle when the hydrogen atom is in its ground state, V_l is purely attractive for e^-—H scattering and purely repulsive for e^+—H scattering. However, as the incident particle approaches, it induces a dipole moment in the atom which in turn leads to an attraction. For large x, the polarization potential seen by the electron is approximately λzy where $z=\mathbf{x}\cdot\mathbf{y}/xy$ and $\lambda=\pm 2/x^2$. We will neglect the higher multipoles. This potential will excite the hydrogen atom to P states and from there to states of angular momentum zero and two. We will only consider s and p states although states of higher l can easily be taken into account. In order to find an approximate form for the hydrogen wave function, we will treat the polarization potential as a perturbation to the electron Hamiltonian

$$H_e=-\nabla_y^2-2/y. \tag{92}$$

The electron part of the trial wave function is then given by

$$q=e^{-y}+\lambda q_1+\lambda^2 q_2+\cdots \tag{93}$$

and the electron energy by

$$E_e=-1+\lambda^2 E_2+\cdots. \tag{94}$$

A simple calculation[33] yields for the p-wave part

$$q_P=\lambda(zy/2)(1+\tfrac{1}{2}y)e^{-y}. \tag{95}$$

For the s-wave part, one finds

$$E_2=-9/8$$

and

$$q_S=[1+C+(\lambda^2y^2/48)(9+3y+\tfrac{1}{2}y^2)]e^{-y},$$

where the d-wave part of q_2 has been dropped. The constant C is determined by the requirement that the trial functions be orthogonal to $|B\rangle$. This gives $C=-1-81\lambda^2/64$. These results suggest that the electron part of the trial function be of the form $P(y)\exp(-ay)$, where a is a variational parameter and $P(y)$ is a polynomial whose coefficients are also variational parameters. Of course, P must be chosen to ensure the proper behavior of the trial function at the origin and to be orthogonal to the bound state. Below the inelastic threshold the trial function must also fall off exponentially for large x, so it is convenient to take the wave function of the scattered particle to be of the form $Q(x)\exp(-bx)$, where Q is also a polynomial in x.

In passing we may note that the second-order correction to the energy, namely,

$$E_e+1=\lambda^2E_2=-(9/2)x^{-4},$$

is just the long-range polarization potential seen by the incident particle.[18]

B. Positronium Formation

In the case of positron-hydrogen scattering, when the energy is sufficiently high, namely, at the first inelastic threshold, it is also possible to produce a final state of positronium in its ground state and a free proton. This is an overlapping resonance situation in which the electron has its choice of being bound on the proton or on the positron. Since these states are degenerate in energy, it is essential in any accurate calculation to include both possibilities. One would be led to try a trial function of the form

$$q_3=\exp[-c|\mathbf{x}+\mathbf{y}|-d|\mathbf{x}-\mathbf{y}|].$$

The variational constant c controls the position of the center of mass of the positronium atom and d controls the relative distance between the electron and the positron. One can improve this trial function by considering the polarization effects in the relative coordinate dependence due to the presence of the nearby proton.

[33] The first-order perturbation calculation was carried out by A. Dalgarno and A. Stewart, Proc. Roy. Soc. (London) **A238**, 269, 276 (1956).

C. Trial Functions and Numerical Results

In order to simplify the calculation, we have chosen the trial functions to be

$$q_S = e^{-bz}\{1-[(a+1)^2/12]y^2\}e^{-ay},$$
$$q_P = zxe^{-bx}ye^{-ay}.$$

Positronium formation was neglected. Since the upper bound potentials contain very attractive central cores, we expect the s-wave trial functions to be very important and to differ from the s wave produced by the long-range polarization potential. Therefore, we have chosen the above functions to represent these effects.

The static potential for electron-hydrogen scattering V_L is purely attractive, but not strong enough to produce a bound state. However, if either the s- or p-state trial function is added, then W_L does become attractive enough to create a bound state. The upper bound potential V_u also has a single bound state, so both the upper and lower bound phase shifts will start out at zero energy from the same point by virtue of Levinson's theorem. Upper and lower bounds on the S wave phase shift for $e^- - H$ scattering obtained from our two trial functions are shown in Fig. 4. The phase shifts for the potentials V_L and V_u are included for comparison. For the scattering length we find

$$5.54 \geq A \geq 1.44.$$

The variational parameters were determined by trial and error. No systematic attempt was made to find the best bounds. It should be recalled that exchange effects have been neglected. The lower bound on the phase shift compares favorably with the results of the strong coupling approximation in which the $1s$, $2s$, and $2p$ states of the hydrogen atom have been taken into account exactly.[18] The result here is $A = 5.04$. However, in the close coupling calculation, it was necessary to solve a three-channel problem exactly whereas we have only solved a single-channel problem.

Calculations have also been performed with the s- and p-state trial functions separately. It turns out that virtual excitation of the hydrogen atom to s states is more important than excitation to p states; that is, the long-range polarization potential is less important than short-range effects. The reason is that the attractive static potential tends to pull the incident electron close to the hydrogen atom where it can induce direct transitions to s states. In view of the simplicity of our trial functions, the results are quite encouraging. With slightly more sophisticated trial functions, it should be possible to obtain quite accurate bounds.

Bounds on the s-wave phase shift for positron-hydrogen scattering have been obtained from the same trial functions that were used for electron-hydrogen scattering. The static potential V_L is purely repulsive, but the addition of the p-state trial function is sufficient to make the upper bound on the scattering length negative (attractive). We find

$$-0.554 \geq A.$$

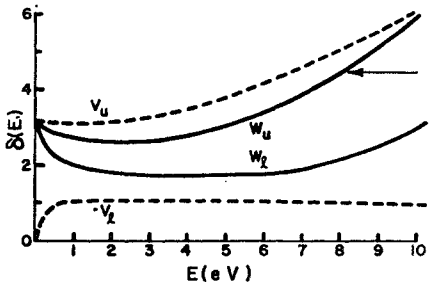

FIG. 4. The s-wave phase-shift bounds for electron-hydrogen scattering neglecting exchange. The exact phase shift must lie between the W_u and W_l lines. The arrow indicates a possible resonance, which must occur above an energy of 8.3 eV. A reasonable extrapolation of the lower limit would predict such a resonance in the vicinity of the inelastic threshold. Also, the s-wave cross section must pass through a zero between 5.4 and 10.2 eV.

Excitation of the hydrogen atom to S states is not important here.

Our lower bounds on the phase shift are again comparable to the results of the closing coupling approximation in which the $1s$, $2s$, and $2p$ states of hydrogen are treated exactly.[18] However, the scattering length here was repulsive. Using fifty trial functions, Schwartz has obtained the essentially exact answer: $A = -2.10$.[14] The main reason for the discrepancy between our result and Schwartz's is undoubtedly our neglect of positronium formation. The positronium channel has the lowest inelastic threshold and therefore should have a large effect on the elastic scattering. In this regard we should note that Spruch has obtained the bound $-1.397 \geq A$,[18] using a simple trial function that takes positronium formation into account.

The upper bound potential V_u is attractive enough to produce a bound state which our simple trial functions can not remove. It is probably necessary to include a trial function which allows for positronium formation in order to obtain a nontrivial upper bound on the scattering length.

VII. CONCLUSIONS AND EXTENSIONS

The most important defect in all approximation schemes hitherto proposed for multiparticle scattering is that one cannot get a reliable estimate of the errors.

The knowledge that an approximation scheme will eventually converge is no comfort when one can only carry out the first few iterations. This is especially true in coupled channel situations. One can produce bound states and/or resonances at very low energies which are due to the forces which act in a channel with a high threshold. Such a channel would tend to be omitted in any first look at the problem. Therefore, the upper and lower bounds on the elastic phase shifts and eigenphase

shifts (which our formalism yields) is crucial in attaining any reasonable accuracy with any reasonable confidence in such cases.

The major results of this paper are the upper and lower variational bounds on the K matrix in multichannel scattering situations. To reiterate, our main theorem rests on the fact that it is possible to imbed the effective potential W_1 into a one-parameter effective potential $W(x)$, such that $W(1)=W_1$ and $W(0)=W_0$, and dW/dx has a fixed sign. Furthermore, we have explicitly constructed solvable W_0's which make dW/dx positive and negative definite. Since the K matrix was proven to be monotonic in $W(x)$, the W_0's provide lower and upper bound phase shifts and K-matrix elements.

It is *not* necessary to know the two-particle wave functions or scattering amplitudes exactly in order to calculate in the three-particle sector. We have explicitly seen this in the electron-hydrogen case. Furthermore, if the energy is such that various two-particle resonances overlap, it is not necessary to form a three-particle wave function by superposing these resonances in an arbitrarily chosen mixture. The variational principles given here automatically choose the optimum combination. Also, by following the variational parameters of the upper and lower bounds from the elastic to the inelastic region, one can be sure of choosing the correct solution of the stationary condition. The difference between the upper and lower bounds then yield a quite reliable estimate of the errors in the inelastic region.

The inelastic effects in pion-pion scattering are known to be very important in determining the position, width, and even existence of the ρ.[34] The attraction caused by the π-ω state evidently allows a meson with the correct mass to bootstrap itself even when the left-hand attraction due to the exchange of a ρ with the *physical* mass is not strong enough to produce a ρ on the right.[35] We plan to return to this problem with our variational bounds and to examine it further. However, it could turn out that the ρ owes its existence to higher mass states, namely to a bound state in the $\bar{N}N$ channel with the 2π state projected out. This bound state would lead to a (shifted) resonance when the π-π channel is coupled in, as we have demonstrated. This argument can be true in spite of any (erroneous) argument about distant singularities being unimportant. Of course, a global bootstrapping approach is still applicable here because the forces which cause the $\bar{N}N$ binding are presumably due to the exchange of π's, ρ's, ω's, etc., all of which will eventually be in the output of such a calculation. This extended Fermi-Yang type model could explain in a reasonable way the nonexistence of low-mass scalar mesons,[36,37] which seem to be an awkward point with the standard bootstrap calculations.[38] This model is now being explored.

In any case, we have proven that the effect of adding more and more inelastic channels to a nonrelativistic problem is to monotonically increase the phase shift in the elastic region. We have further demonstrated that our methods can be actually applied in practice by considering the nontrivial example of electron-hydrogen and positron-hydrogen scattering. We consider this example to be a typical high-energy calculation. The numerical bounds on the s-wave phase shifts were quite good considering the simplicity of our trial functions. More work on this problem, especially in the energy region just below the inelastic threshold and including exchange effects, seems to be called for.

It has been clear for some time that the unitarity corrections to the peripheral model are large, and tend to narrow the diffraction width by absorbing the low partial waves.[39] These corrections have the same effect as the "form factors" which are added to the peripheral model to get agreement with experiment. These factors are interpreted as off-mass-shell effects, but are usually much too rapidly varying to be reasonably interpreted in such a manner. We hope to return to this interesting point after our approach has been extended to the relativistic problem.

We would like to make a remark concerning the general approach to existence proofs for the scattering equation. The first point is that the Hilbert-Schmidt approach seems to have little to do with the type of kernel occurring in the scattering equation. The main point here is the fact that even with the optimum local similarity transformation, the Hilbert-Schmidt norm is independent of the energy along the positive real axis. However, we know that as the energy increases, the Fredholm determinant approaches unity and eventually, for sufficiently high energy, the Born series converges. The H-S norm gives no hint of such a behavior. Therefore, it cannot be the *best* bound, nor the best way to approach the problem.

Progress in this direction has been made by Rubin[40] who has been able to avoid the difficulties with real energies by continuing the inner product integral paths. This approach avoids the introduction of a Banach space as was used by Hunziker.[41] This latter procedure does not seem to clarify the physics of the problem. Also, Rubin's method seems to be extendable to the three-body problem[42] and to the relativistic Bethe-Salpeter case.[43]

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[34] R. Blankenbecler, Phys. Rev. **125**, 755 (1962).

[35] F. Zachariasen and C. Zemach, Phys. Rev. **128**, 849 (1962).

[36] We thank M. Goldberger for bringing up this important question and for illuminating discussions.

[37] Preliminary estimates based on this model seem to lead to octets of positive parity scalar, vector, and tensor mesons. Their masses are in the neighborhood of 1000–1450 MeV, with the scalar particles tending toward the higher figure. It should be possible to see these vector and tensor mesons at such an energy, but the scalars will be more difficult.

[38] See, for example, the bootstrap-unitary symmetry calculation of C. Hong-Mo, P. DeCelles, and J. E. Paton, Nuovo Cimento (to be published).

[39] M. Baker and R. Blankenbecler, Phys. Rev. **128**, 415 (1962).

[40] M. Rubin (to be published).

[41] W. Hunziker, Helv. Phys. Acta **34**, 593 (1961).

[42] W. Hunziker and M. Rubin (private communication).

[43] G. Tiktopoulos (to be published).

To return to the upper and lower variational bounds on the K matrix elements, we feel that our approach will have applications in many unsolvable problems—that is, those problems which cannot be solved on a finite computer. Among these applications are atomic and molecular collisions, models for nuclear reactions, many-body problems, the relativistic Bethe-Salpeter equation, and to dispersion relations. We plan to pursue some of these problems later.

Finally, we would like to stress the importance of the pioneering work of Spruch and his collaborators on variational principles. Even though our upper and lower bounds are quite distinct and independent, and bear little relation to the lower bound principle of Spruch, his work suggested several points which were included in our discussion.

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Theorem on Separation of Variables with Application to Static-Source Meson Theory

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A general formulation is given of the process by means of which one eliminates certain redundant degrees of freedom occurring in interacting quantum-mechanical systems. This may be considered a generalization of the transformation to center of mass in problems having translational invariance. When applied to the pion-nucleon system, the static-source approximation arises as the first term in a series, the higher terms of which are easily calculable using an algorithm developed in the Appendix. Thes system is not an expansion in the inverse mass of the nucleon, and it is shown that the static source approximation need not be considered as a nonrelativistic approximation.

INTRODUCTION

IN energy eigenvalue problems involving interacting systems and possessing translational invariance, one usually transforms to center-of-mass coordinates, eliminates redundant degrees of freedom, and consequently obtains an equivalent problem in a reduced Hilbert space. It is not surprising that such a reducibility exists whenever interacting systems possess an Abelian invariance group. A general procedure by which such reductions may be effected is discussed in Sec. II. Section III contains a heuristic example.

Of some interest may be the simple field-theoretic examples in Sec. IV and V. It is demonstrated, using a hypothetical heavy boson-light boson interacting system and the nucleon-pion system, how such interacting-field theories lead straightforwardly to an approximation expansion the first term of which is a "static source" theory. No statements about "nonrelativistic approximations" are made. Succeeding terms in the series are easily obtained using an algorithm developed in the Appendix.

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II. ELIMINATION OF DEGREES OF FREEDOM ASSOCIATED WITH CONSERVED ADDITIVE QUANTUM NUMBERS

Consider an energy eigenvalue problem in a Hilbert space which can be decomposed into the form

$$\mathfrak{C}=\mathfrak{C}_j\otimes\tilde{\mathfrak{C}}. \tag{1}$$

Let H be the Hamiltonian of the system and let

$$J=j+\tilde{j};\quad J=\{J_1, J_2, \cdots\} \tag{2}$$

be a set of operators such that

$$[H,J]=0 \tag{3}$$

and such that the j are a complete commuting set for $\mathfrak{C}_j$. Let some appropriate complete commuting set for $\tilde{\mathfrak{C}}$ be denoted by k. One can then use the following notation[1]:

$$|j'\rangle\epsilon\mathfrak{C}_j;\quad |k'\rangle\epsilon\tilde{\mathfrak{C}};\quad |j',k'\rangle\epsilon\mathfrak{C}. \tag{4}$$

Let $|\psi\rangle$ be the simultaneous eigenstate in $\mathfrak{C}$ of H and the J,

$$H|\psi\rangle\equiv H'|\psi\rangle;\quad J|\psi\rangle\equiv J'|\psi\rangle. \tag{5}$$

[1] Primed symbols will always denote eigenvalues of corresponding operators.