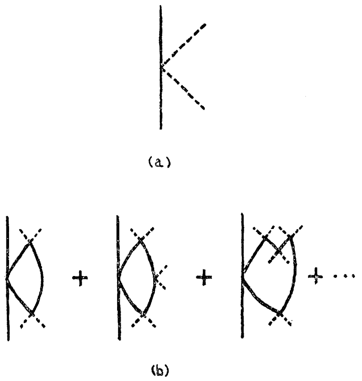

FIG. 1. Perturbation terms for $T=0$. Dashed lines correspond to zero-momentum particles, solid lines to excited particles.

two-body potential, we obtain for ϵ_k

$$\epsilon_k^2=(k^2/2m)^2+N_0V_{\mathbf{k}}k^2/m. \tag{3.2}$$

For the charged boson gas with a uniform positive background,

$$V_{\mathbf{k}}=4\pi e^2/k^2v,\quad \mathbf{k}\neq 0,\\ \quad =0,\quad \mathbf{k}=0, \tag{3.3}$$

where v is the volume of the system, and it appears that we obtain an energy gap for $\mathbf{k}\to 0$. This results from taking Σ's which are not well behaved at the origin, namely,

$$\lim_{\mathbf{k}\to 0} V_{\mathbf{k}}\neq V_0.$$

Thus, the energy gap is probably a result of the approximations. The uniform positive background model leads directly to this discontinuity and the replacement of this by discrete positive charges will remove it. Further, higher approximations to the Σ's may not have the $1/k^2$ dependence for low k.

Lastly, we notice that the importance of using factors N_0 rather than N in Eq. (3.1) has often been stressed. It is, however, easy to see that the sum of all diagrams like those in Fig. 1(b) contributing to $\Sigma_{11}(\mathbf{k},\omega)$ give us $2N'V_0$ for low values of $\mathbf{k}$ and ω approximately, whereas the diagram in Fig. 1(a) gives us $N_0(V_0+V_{\mathbf{k}})$, the contribution we have already included in Eq. (3.1), giving a total contribution of $2NV_0$. A similar argument can be applied for $\Sigma_{11}{}^{\beta}(\mathbf{k},\omega)$ at nonzero temperatures. For slowly varying potentials it may, therefore, be a better approximation to put

$$\Sigma_{11}{}^{\beta}(\mathbf{k},\omega)=N(V_0+V_{\mathbf{k}}).$$

Similar considerations could apply if we replaced $V_{\mathbf{k}}$ by a reaction matrix element. There is no analogous argument for Σ_{02}. A reasonable model for discussing the condensed boson gas at temperatures different from zero might be to assume that Σ_{11} was independent of temperature and that Σ_{02} depended on the temperature solely through its factor of N_0.

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Static Approximation and Bounds on Single-Channel Phase Shifts*†

YUKAP HAHN, THOMAS F. O'MALLEY, AND LARRY SPRUCH
Physics Department, New York University, New York, New York

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A single-channel scattering process with the set of quantum numbers C is completely characterized by a phase shift, η_C. A common approximation in the determination of η_C for the scattering of a particle by a compound system is to assume that, apart from the possibility of an exchange of the incident particle with an identical target particle, the target is unaffected by the incident particle. The incident particle is then scattered by the static potential generated by the target in its ground state. The phase shift determined in this approximation, to be called $\eta_C{}^P$, can be calculated for a number of scattering processes. Let H represent the Hamiltonian of the entire system, incident particle plus target, let E_{T0} be the ground-state energy of the target, and let $E'_C{}^Q$ be the smallest energy for which $E'_C{}^Q+E_{T0}-H$ is a negative definite operator in the space in which the given quantum numbers are C and in which the ground state of the target is projected out. Utilizing the generalized optical potential formalism due to Feshbach and others, it can then be shown that $\eta_C>\eta_C{}^P$ if the incident energy is less than $E'_C{}^Q$. (The bound is probably valid for higher energies, perhaps for all energies for which the process remains a single-channel process. If so, however, the difference between η_C and $\eta_C{}^P$ for these higher energies will generally be large, of the order of a multiple of π, and the bound will not be immediately useful. We will, therefore, be concerned primarily with incident energies E' less than $E'_C{}^Q$.) Furthermore, as one allows for more and more virtual excitation of the target system, the approximate phase shift is guaranteed to improve if E' is less than $E'_C{}^Q$, and $E'_C{}^Q$ will itself increase. Applications are given to the scattering of electrons and of positrons by hydrogen atoms.

1. INTRODUCTION

THE minimum principle formulation for the determination of the scattering length in single-channel scattering[1,2] has most of the properties that one would want to have. At nonzero incident energies, however, the minimum principle formulation for the

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† A preliminary report of this work was given at the New York Meeting of the American Physical Society [Bull. Am. Phys. Soc. **7**, 41 (1962)].

[1] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959); **117**, 1095 (1960).

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

determination of the phase shift in single-channel scattering and of the elements of the reactance matrix for multichannel scattering requires[3] truncation of some of the potentials and the erection of potential barriers, with the consequence that the complexity of the calculation can be very much increased. There is an alternate method[4] which can provide upper and lower variational bounds at zero or nonzero energies, but this latter method requires among other things the evaluation of matrix elements of H^2, where H is the Hamiltonian, and can therefore also be quite cumbersome. It would be very useful to have a minimum principle valid at nonzero energies that did not require any artificial tampering with the potentials and that did not require the evaluation of matrix elements of H^2. We will not in this paper present such an improved minimum principle, but as a preliminary to doing so, and because it is of interest in its own right, we will show that a bound on the phase shift for single-channel scattering can often be obtained by a method which does not require the evaluation of matrix elements of H^2 and which treats the true potential.

We will be concerned with the case for which the incident particle, the target, and the energy are such that elastic scattering is the only possible process and such that the scattering can be decomposed in some *a priori* way, through conservation of angular momentum for example, into uncoupled channels. When the incident particle is distinguishable from the target particles, a standard approximation in the study of such single-channel processes is the static or one-body approximation, in which it is assumed that the target system remains in its ground state throughout the scattering process. In this approximation, the problem reduces to the one-body problem in which the incident particle is scattered by the static potential generated by the target in its ground state. For an incident relative energy $E'=\hbar^2k^2/2\mu$, where μ is the reduced mass, the static approximation phase shift for angular momentum L will be denoted by $\eta_L{}^P(k)$; the index L and the argument k will, however, often be omitted. When the incident particle is indistinguishable from some of the target particles, the possibility of exchange must be taken into account, and the approximation analogous to that described above is sometimes again referred to as the static approximation and sometimes as the static exchange approximation. We will use the phrase static approximation to describe both the distinguishable and indistinguishable cases.

Among the many scattering problems that satisfy the requirements that we have imposed are the scattering of positrons by hydrogen atoms at energies below $\frac{1}{2}(13.6)$ eV, to avoid the possibility of pickup, and the scattering of electrons by hydrogen atoms at energies below $\frac{3}{4}(13.6)$ eV, to avoid the possibility of excitation. The possibility of electron-positron annihilation is ignored in e^+H scattering, and the possibility of radiative capture is ignored in e^-H scattering. (The interaction with the radiation field will be ignored throughout.) For fixed energy, there is one phase shift for each value of L for e^+H scattering, and there are two phase shifts, a triplet and a singlet phase shift, for each value of L for e^-H scattering. What makes the above two examples of particular interest is that the true phase shifts for $L=0$, $\eta_0(k)$, are known with considerable precision for a range of values of k. The values of $\eta_L{}^P(k)$ can be calculated to practically arbitrary precision and many calculations of very high precison have been performed.[5] To our knowledge the observation has not previously been made, but an examination of the data shows that $\eta_0(k)\geq\eta_0{}^P(k)$ for all cases for which both phase shifts are known. It will be the primary purpose of the present paper to give some insight into the origins of this inequality and to delineate as precisely as possible the conditions on L and on k under which this inequality can be expected to hold for the e^-H and e^+H problems, and for other problems. (The methods to be discussed are not in any sense limited to atomic scattering problems.) The question is of some interest for the static approximation is an extremely simple one and a knowledge that $\eta_L{}^P(k)$ provides a bound on $\eta_L(k)$ can be very valuable.

Furthermore, with the advent of high-speed computers, it has become feasible to solve to more or less arbitrary precision the problem for which the less restrictive approximation is made that during the scattering process the target can be in its ground state or can be virtually excited to one of m excited states, where for present computers m should not be more than perhaps 5, and where the states would generally be taken to be low-lying states. Examination of the numerical results[5] for e^-H and e^+H scattering shows that the results improve as one introduces additional states, and that the results remain below the true value. This point will also be discussed.

The basic equation in our approach is Eq. (2.14) [or its equivalent, Eq. (2.26′)]. This equation, which contains a generalized optical potential, represents the equivalent one-body scattering problem. (The potential is, in fact, often referred to as the equivalent potential.) The equation is of considerable importance, particularly in nuclear physics, because it provides the theoretical foundation for the optical model. Furthermore, one can use the same approach to derive the resonant aspects of scattering *without* having to introduce a channel radius,

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[3] L. Rosenberg and L. Spruch, Phys. Rev. **120**, 474 (1960); **121**, 1720 (1961); **125**, 1407 (1962).

[4] T. Kato, Progr. Theoret. Phys. (Kyoto) **6**, 394 (1951); L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960); R. Bartram and L. Spruch, J. Math. Phys. **3**, 287 (1962).

[5] A very nice review of the work that has been done on low-energy scattering of electrons and positrons by hydrogen atoms is contained in a paper by P. G. Burke and K. Smith, Revs. Modern Phys. **34**, 464 (1962). This paper gives the formulation of the static approximation and of the improved approximations in which some low-lying hydrogenic states are included, as well as the numerical results that have been obtained.

that is, without having to truncate the potentials. The equation has been derived by a number of people.[6,7] Our notation follows that of Feshbach most closely.

2. STATIC APPROXIMATION—INCIDENT PARTICLE DISTINGUISHABLE

The simpler case for which the incident particle is distinguishable from all of the target particles will be considered first. For purposes of simplicity, it will be further assumed that the incident particle is spinless and that the total angular momentum of the ground state of the target is zero. The method can be readily generalized to a much wider class of problems. It is obviously generalizable to e^+H scattering for which the spins of the electron, of the positron, and of the proton play no role. It can also be applied to the scattering of a particle of spin $\frac{1}{2}$ by a target whose ground state has a total angular momentum of zero, where the interaction of the incident and target particles can include spin-spin and tensor forces. Finally, though all of our considerations will be limited to the case for which there is no Coulomb interaction, there would be no difficulty in extending the results to include that interaction.

Let $\mathbf{q}$ represent the coordinate of the incident particle relative to the center of mass of the target and let $\mathbf{r}$ represent the spatial and possibly the spin and isotopic spin coordinates of the target particles. The total Hamiltonian and total energy of the entire system, target plus incident particle, will be denoted by H and E, respectively. The ground state of the target has a wave function $\psi_{T0}(\mathbf{r})$ and an energy E_{T0}. $E'=E-E_{T0}=\hbar^2k^2/2\mu$ will then be the relative incident energy. The excited state wave functions and energies of the target will be denoted by $\psi_{T1}(\mathbf{r}), \psi_{T2}(\mathbf{r}), \cdots$ and $E_{T1}, E_{T2}, \cdots$, respectively. By assumption, E lies below E_{T1}, or equivalently E' lies below E_{T1}-E_{T0}, so that excitation is not energetically possible. It may be necessary to impose more severe restrictions on E in order to eliminate other processes, such as pickup, for we are concerned throughout only with single-channel processes.

The regular solution $\Psi_L(\mathbf{r},\mathbf{q})$ of

$$(H-E)\Psi_L(\mathbf{r},\mathbf{q})=0, \tag{2.1}$$

which satisfies the boundary condition that as $q\rightarrow\infty$,

$$\Psi_L(\mathbf{r},\mathbf{q})\rightarrow\psi_{T0}(\mathbf{r})P_L(\cos\Theta)\sin(kq-\tfrac{1}{2}L\pi+\eta_L)/q \tag{2.2}$$

determines the phase shift η_L to within a multiple of π. Θ is the angle between $\mathbf{q}$ and some fixed axis.

We now introduce two projection operators, P and Q, which operate in the space of the target particle coordinates. P is defined by its operation on an arbitrary function $f(\mathbf{r},\mathbf{q})$,

$$Pf(\mathbf{r},\mathbf{q})=|\psi_{T0}\rangle\langle\psi_{T0}|f=\psi_{T0}(\mathbf{r})\int\psi_{T0}(\mathbf{r}')f(\mathbf{r}',\mathbf{q})d\mathbf{r}', \tag{2.3'}$$

that is, P projects onto the ground state of the target, while Q projects onto all of the excited states of the target, including the continuum states. The operator $P+Q$ is then the unit operator, and we can rewrite Eqs. (2.1) and (2.2) as

$$(P+Q)(H-E)(P+Q)\Psi_L{}^{P+Q}=0, \tag{2.4}$$

$$\Psi_L{}^{P+Q}\rightarrow\psi_{T0}(\mathbf{r})P_L(\cos\Theta)\times\sin(kq-\tfrac{1}{2}L\pi+\eta_L{}^{P+Q})/q, \tag{2.5}$$

where there is no difference between $\Psi_L{}^{P+Q}$ and Ψ_L nor between $\eta_L{}^{P+Q}$ and η_L. The superscript notation is unnecessary for present purposes, but will prove to be convenient when some virtual excitation is allowed. (See Sec. 4.)

Since P and Q operate in orthogonal spaces, Eq. (2.4) can be rewritten as the pair of coupled equations

$$P(H-E)(P+Q)\Psi_L{}^{P+Q}=0, \tag{2.6}$$

$$Q(H-E)(P+Q)\Psi_L{}^{P+Q}=0. \tag{2.7}$$

(The latter equation is, of course, itself equivalent to an infinite set of coupled equations.) $\Psi_L{}^{P+Q}$ can be written in the form

$$\Psi_L{}^{P+Q}=\textstyle\sum_i\psi_{Ti}(\mathbf{r})u_i(\mathbf{q}), \tag{2.8}$$

where, as $q\rightarrow\infty$,

$$u_0(\mathbf{q})\rightarrow[\sin(kq-\tfrac{1}{2}L\pi+\eta_L{}^{P+Q})/q]P_L(\cos\Theta), \tag{2.9}$$

and where, for $i\neq0$, $u_i(\mathbf{q})$ vanishes more rapidly than $1/q$. The L dependence of the u_i has been suppressed. We then have that

$$Q\Psi_L{}^{P+Q}=\textstyle\sum'_i\psi_{Ti}(\mathbf{r})u_i(\mathbf{q}), \tag{2.10}$$

where the prime indicates, here and later, that the sum is to be taken over the excited states only. It follows that $Q\Psi_L{}^{P+Q}$ vanishes more rapidly than $1/q$ as $q\rightarrow\infty$ and that the continuum portion of QHQ begins not at E_{T0}, as does that of H, but at E_{T1}. QHQ may also have some discrete eigenvalues below E_{T1}; if there exist $N_L{}^Q$ orthonormal states of total angular momentum L which satisfy

$$Q(H-E_{Ln}{}^Q)Q\Phi_{Ln}{}^Q=0,\ n=1,\cdots,N_L{}^Q, \tag{2.11}$$

with $E_{Ln}{}^Q<E_{T1}$, the spectrum of QHQ in the space of total angular momentum L will include the $N_L{}^Q$ discrete eigenvalues $E_{Ln}{}^Q$. The spectrum of $Q(H-E)Q$ in the space of total angular momentum L will then include the $N_L{}^Q$ discrete eigenvalues $E_{Ln}{}^Q-E$ and the continuum bounded from below by the positive value $E_{T1}-E$. (See Fig. 1.)

Ignoring the set of measure zero probability that any of the $E_{Ln}{}^Q$ are equal to E, it follows then that there is no solution Ψ_{hom} of the homogeneous equation

$$Q(H-E)Q\Psi_{\text{hom}}=0, \tag{2.12}$$

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[6] H. Feshbach, Ann. Phys. (New York) **5**, 357 (1958); see also H. Feshbach, in Ann. Rev. Nuclear Sci. **8**, 44 (1958).

[7] L. Fonda and R. G. Newton, Ann. Phys. (New York) **10**, 490 (1960). Also, G. Breit, Phys. Rev. **58**, 506 and 1069 (1940), **69**, 472 (1946), B. Zumino, New York University, Courant Institute of Mathematical Sciences, Research Report No. CX-23, March, 1956 (unpublished) contain related materials.

which vanishes more rapidly than $1/q$ as $q\rightarrow\infty$. The inversion of $Q(H-E)Q$ is then unique, and Eq. (2.7) can be rewritten as

$$Q\Psi_L{}^{P+Q}=\frac{1}{Q(E-H)Q}QHP\Psi_L{}^{P+Q}. \tag{2.13}$$

If we substitute this equation into Eq. (2.6), we arrive at

$$P\left[H+HQ\frac{1}{Q(E-H)Q}QH-E\right]P\Psi_L{}^{P+Q}=0. \tag{2.14}$$

Equation (2.14) still depends upon $\mathbf{r}$ as well as $\mathbf{q}$, but in fact the $\mathbf{r}$ dependence appears only through the presence of a factor $\psi_{T0}(\mathbf{r})$ on the left, which can be dropped. Equation (2.14) is therefore a one-body problem, entirely equivalent to the original problem, in which the effects of virtual excitation are taken into account through the presence of the term

$$PHQ\frac{1}{Q(E-H)Q}QHP. \tag{2.15}$$

The factor QHP represents virtual excitation from the ground state, the central factor represents propagation in the excited states, and the factor PHQ represents de-excitation. Due to the central factor the expression is only a formal one but it is elegantly compact.

In the static approximation, one introduces a function

$$\Psi_L{}^P(\mathbf{r},\mathbf{q})=\psi_{T0}(\mathbf{r})u_0{}^P(\mathbf{q}), \tag{2.16$'$}$$

which is defined as the regular solution of

$$P(H-E)P\Psi_L{}^P=0, \tag{2.17}$$

for which

$$u_0{}^P(\mathbf{q})\rightarrow[\sin(kq-\tfrac{1}{2}L\pi+\eta_L{}^P)/q]P_L(\cos\Theta). \tag{2.18}$$

The only difference between the definitions of η_L and of $\eta_L{}^P$ is then the presence of the operator (2.15) in expression (2.14).

Now it is well known[8] for potential scattering that if $V^{(1)}(r)$ and $V^{(2)}(r)$ are real potentials which are not too singular at the origin and fall off sufficiently rapidly to define (real) phase shifts $\eta^{(1)}$ and $\eta^{(2)}$ for specified energy and angular momentum, and if $V^{(1)}(r)\leq V^{(2)}(r)$ for all r, then $\eta^{(1)}\geq\eta^{(2)}$. The proof of the monotonicity theorem carries through in precisely the same way for nonlocal potentials as for local potentials for all normal situations. (For esoteric situations such as a bound state embedded in the continuum, it may be necessary to explicitly assume the phase shift to be a continuous function of the strength of the potential. See Appendix B.) It follows that if the operator given by expression (2.15) is negative definite, then $\eta_L(k)>\eta_L{}^P(k)$. Since

$$(\chi_L,\ PHQ[Q(E-H)Q]^{-1}QHP\chi_L) \\ =(QHP\chi_L,\ [Q(E-H)Q]^{-1}QHP\chi_L), \tag{2.19}$$

where χ_L is a normalizable function and has a total angular momentum of L but is otherwise arbitrary, the phase shift inequality will necessarily be valid if $[Q(E-H)Q]^{-1}$ is negative definite in the space of total angular momentum L. Finally, since an operator is negative definite if its reciprocal is, we have our basic result, that $\eta_L(k)>\eta_L{}^P(k)$ if $Q(E-H)Q=Q(E'+E_{T0}-H)Q$ is negative definite in the space of total angular momentum L.

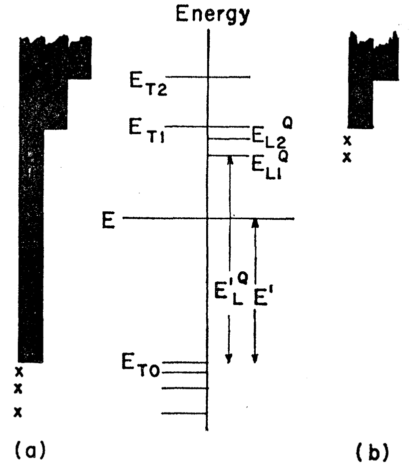

FIG. 1. Schematic plot of the spectra of (a), the total Hamiltonian H, and of (b), the Hamiltonian QHQ in which the ground state of the target has been projected out, in the space of angular momentum L. E_{T0} and the E_{Ti} for $i>0$ are the ground state and excited state energies (of all angular momenta) of the target. E is the total energy of the system and E' is the incident relative kinetic energy. For $E'<E'_L{}^Q$, the static approximation phase shift $\eta_L{}^P(k)$ can be guaranteed to provide a lower bound on the exact phase shift $\eta_L(k)$, a lower bound which can generally be expected to be within π of $\eta_L(k)$.

From our definition of the $E_{Ln}{}^Q$, it follows that $E'_L{}^Q\equiv E_{L1}{}^Q-E_{T0}$ is the greatest value of E' for which $Q(E'+E_{T0}-H)Q$ is negative definite in the space of total angular momentum L. Our basic result can then be restated as follows:

$$\eta_L(k)>\eta_L{}^P(k)\quad\text{if}\quad E'<E'_L{}^Q. \tag{2.20}$$

In arriving at (2.20), we need not fix the arbitrary multiple of π in the definition of $\eta_L{}^P$. The particular choice of the multiple that is made is irrelevant, for it is only the difference between the phase shifts that appears in the inequality, and the difference is uniquely determined by studying the (continuous) change in the phase shift as the interaction in expression (2.15) is slowly turned on.

We cannot hope to actually determine $E'_L{}^Q$, but we can hope to find a lower bound on $E'_L{}^Q$, and if E' were less than the lower bound it would certainly be less than

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[8] This theorem has been known for years but does not appear in any of the standard texts. For a proof for local potentials, see L. Spruch, in *Lectures in Theoretical Physics, Boulder, 1961*, edited by W. E. Brittin and W. B. Downs [Interscience Publishers, Inc., New York (to be published)], Vol. 4.

$E'_L{}^Q$. It is of course unfortunately true that no general method exists for finding a lower bound on the energy of a many-body problem, let alone a lower bound that can lead to useful results. For e^-H scattering, however, the determination of a useful lower bound is a triviality. (This will be shown in Sec. 3. The question of the negative definiteness of $Q(E-H)Q$, with Q somewhat differently defined, will also arise when there are identical particles.) The determination of a useful lower bound does not appear to be so simple for e^+H scattering; at the sacrifice of rigor, one can use reasonability arguments there.

Equation (2.14) can be put into a slightly less abstract form. With the motion of the center of mass subtracted out, we write

$$H=H(\mathbf{r},\mathbf{q})=H_T(\mathbf{r})+T(\mathbf{q})+V(\mathbf{r},\mathbf{q}), \qquad (2.21)$$

where $H_T(\mathbf{r})$ represents the target Hamiltonian, $T(\mathbf{q})$ the kinetic energy operator of the relative motion of the incident particle and the center of mass of the target, and $V(\mathbf{r},\mathbf{q})$ the interaction of the incident particle and the target particles. Since

$$H_TP=PH_T=E_{T0}P, \qquad (2.22')$$

we have

$$PHQ=PVQ, \quad QHP=QVP, \qquad (2.23)$$

and Eq. (2.14) becomes

$$\left(T+V_{00}+PVQ\frac{1}{Q(E-H)Q}QVP-E'\right)P\Psi=0. \qquad (2.24')$$

where

$$V_{ij}=V_{ij}(\mathbf{q})=\int\psi_{Ti}^*(\mathbf{r})V(\mathbf{r},\mathbf{q})\psi_{Tj}(\mathbf{r})d\mathbf{r}=V_{ji}^*, \qquad i=0,1,2, \qquad (2.25')$$

Introducing the column vector $\mathbf{V}_0$, with elements V_{10}, V_{20}, $\cdots$, and dropping an irrelevant factor $\psi_{T0}(\mathbf{r})$, we can write

$$\left(T+V_{00}+\mathbf{V}_0{}^\dagger\frac{1}{E-\mathbf{H}}\mathbf{V}_0-E'\right)u_0=0, \qquad (2.26')$$

where

$$H_{ij}=V_{ij}(\mathbf{q})+[T(\mathbf{q})+E_{Ti}]\delta_{ij}, \quad i\geq 1, \quad j\geq 1. \qquad (2.27')$$

The potential

$$\mathcal{V}=V_{00}+\mathbf{V}_0{}^\dagger\frac{1}{E-\mathbf{H}}\mathbf{V}_0 \qquad (2.28')$$

which appears in Eq. (2.26) is referred to as the generalized optical potential. It is clear since the problem under consideration is a single-channel process with a real phase shift that $\mathcal{V}$ is real and that $\mathcal{V}$ falls off sufficiently rapidly so that a phase shift can be defined. ($\mathcal{V}$ will fall off only as $1/r^4$ for the scattering of a charged particle by a neutral polarizable system, for electron scattering by a neutral atom, for example, but that is fast enough.)

There is one last formulation which we would like to record here, even though it is equivalent to those already given, because it will be useful when we come to the scattering of nucleons by nuclei. We substitute the expansion for Ψ as given by Eq. (2.8) into $(H-E)\Psi=0$, with H given by Eq. (2.21), and take the inner product with ψ_{Tj}. We arrive immediately at

$$[T+V_{jj}-(E-E_{Tj})]u_j=-\textstyle\sum_{i\neq j}V_{ji}u_i. \qquad (2.29)$$

Isolating the equation for $j=0$, the u_i for $i\neq 0$ can be eliminated and we arrive at Eq. (2.26′).

Energies above "Resonance"

We have just seen that $\eta_L{}^P$ is less than η_L if E' is less than $E'_L{}^Q$. The question remains as to how the two phase shifts compare for incident energies greater than $E'_L{}^Q$. The question will of course not arise unless there exist "bound state" eigenfunctions $\Phi_{Ln}{}^Q$ of $Q(H-E)Q$ with energies $E_{Ln}{}^Q$ less than E_{T1}.

An equation of the form of Eq. (2.24′) is still valid even if eigenfunctions $\Phi_{Ln}{}^Q$ do exist, but in that case the factor $[Q(E-H)Q]^{-1}$ will contain terms of the form

$$\frac{|\Phi_{Ln}{}^Q\rangle\langle\Phi_{Ln}{}^Q|}{E-E_{Ln}{}^Q}.$$

We have not made a thorough investigation of the matter, but it seems rather certain that the effect of any one such term, if $E_{Ln}{}^Q$ is "sufficiently far away" from any other energy eigenvalues, is to increase the true phase shift by an amount of the order of π as the energy changes from a value somewhat below $E_{Ln}{}^Q$ to a value somewhat above.[9] Since the value of the static approximation will not change appreciably in this energy interval, the inequality relationship between the exact and static approximation phase shifts will remain valid.

The inequality may well remain valid even when there are eigenvalues rather close together. We will not pursue this any further, however, for the question as to whether η_L remains above $\eta_L{}^P$ for incident energies above $E'_L{}^Q$ is not of very great interest from the present point of view, even for isolated "resonances." The reason is that the difference between the exact and static approximation phase shifts will then be of the order of a multiple of π and since contributions to the cross section involve the sine of the phase shift, the knowledge that $\eta_L{}^P$ provides a bound on η_L will not give any immediately useful information about η_L.[10]

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[9] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics*, (John Wiley & Sons, Inc., New York, 1952), pp. 398–404.

[10] The present paper can be thought of as providing an extension to incident energies other than zero of a theorem obtained by L. Spruch and L. Rosenberg, Nuclear Phys. **17**, 30 (1960) on the exact and static approximation scattering lengths, A and A^P. The theorem states that A^P provides an upper bound on A if the static approximation gives the correct number of composite bound states. If there are fewer composite bound states, η will almost

The realization that the bound may well be valid at all energies below excitation is nevertheless useful in that it provides some insight into the methods of the minimum principle for the phase shift, for there one of the major steps that has to be taken is to "subtract out" the effects of any of the "resonances" that occur at energies lower than that under consideration.

We have nothing further to say about incident energies above $E'_L{}^Q$ in the present paper. It should however be made clear that any proofs of the existence of a bound for incident energies less than $E'_L{}^Q$ are not to be taken to imply that the bound is necessarily false above $E'_L{}^Q$.

3. STATIC APPROXIMATION—INCIDENT PARTICLE INDISTINGUISHABLE

A. Two Fermions and a Center of Force

We will begin by considering the scattering of a fermion by an identical fermion bound to a center of force. A prototype problem is the scattering of an electron by a hydrogen atom, and for simplicity the method will be discussed in terms of that problem. The only effect of the spins of the two electrons is to impose the restriction that the scattering wave function be either symmetric or antisymmetric in the spatial coordinates of the two electrons.

We will again introduce a projection operator P, but the choice of P is not now quite as obvious as it was for distinguishable particles. To begin with, P must clearly treat the two electrons on an equal footing. More significantly, the choice of P and of Q must be such that $Q(E-H)Q$ is a negative-definite operator in the space of the given angular momentum for a significant range of values of E. The values of E that are of present interest are from $E=E_{T0}=-13.6$ eV, for $E'=0$, to $E=\frac{1}{4}E_{T0}=-3.4$ eV, for $E'=10.2$ eV, the threshold for excitation. The continuous spectrum of QHQ must therefore be bounded from below by a value greater than -13.6 eV if we are to obtain any useful results. It follows that *neither* electron can be in the 1*s* (ground) state. We therefore choose $Q=Q_1Q_2$, where Q_k for $k=1$ or 2 is a projection operator in the space of the kth electron which projects onto any one of the excited hydrogenic states. Letting P_k for $k=1$ or 2 be the ground-state projection operator in the space of the kth electron, so that $P_k=1-Q_k$, P is then given by

$$P=P_1+P_2-P_1P_2. \tag{3.1}$$

TABLE I. Lower bounds on $E'_L{}^Q$ for the scattering of electrons by hydrogen atoms for all values of L and for the singlet and triplet cases. For incident energies less than this lower bound, the static approximation phase shift is guaranteed to provide a lower bound on the exact phase shift. These bounds are rigorous but they can be crude because the e^2/r_{12} term was ignored. The value 8.7 eV, in parentheses, was obtained by a more detailed calculation in which the effect of the e^2/r_{12} term was partially taken into account.

L	Symmetry	Lowest states	Lower bound on $E'_L{}^Q$ (eV)
0	singlet	$(2s)^2$ or $(2p)^2$	6.8 (8.7)
0	triplet	$(2s)(3s)$ or $(2p)(3p)$	8.7
1	either	$(2s)(2p)$	6.8
2	singlet	$(2p)^2$	6.8
2	triplet	$(2s)(3d)$ or $(2p)(3p)$	8.7
>2	either	$(2p)(n=L,\ l=L-1)$	$(\frac{3}{4}-1/L^2)13.6$

P is therefore one if either or both electrons are in the 1*s* state and is zero otherwise. More formally, the effects of P and of Q can also be described as follows. Given a function $\Phi(\mathbf{r}_1,\mathbf{r}_2)$ which has a specified symmetry and a specified angular momentum but which is otherwise arbitrary, we can write

$$\Phi(\mathbf{r}_1,\mathbf{r}_2)=\pm\Phi(\mathbf{r}_2,\mathbf{r}_1)=\textstyle\sum_i \Phi_i(\mathbf{r}_1,\mathbf{r}_2), \tag{3.2}$$

where

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2)=\psi_{Ti}(\mathbf{r}_1)\varphi_i(\mathbf{r}_2)\pm\psi_{Ti}(\mathbf{r}_2)\varphi_i(\mathbf{r}_1). \tag{3.3}$$

The φ_i are not uniquely defined by specification of the Φ_i. (An interesting consequence of this fact is obtained in Appendix A.) Without loss of generality, the φ_i for $i\neq 0$ can be chosen to be orthogonal to ψ_{T0}. With this choice of the φ_i, we have

$$P\Phi=\Phi_0,\quad Q\Phi=\textstyle\sum' \Phi_i, \tag{3.4}$$

where here as elsewhere the restricted sum, denoted by the prime, excludes $i=0$.

Since

$$H(\mathbf{r}_1,\mathbf{r}_2)=H_{\text{hyd}}(\mathbf{r}_1)+H_{\text{hyd}}(\mathbf{r}_2)+V(|\mathbf{r}_1-\mathbf{r}_2|), \tag{3.5}$$

where

$$H_{\text{hyd}}(\mathbf{r})=T(\mathbf{r})-e^2/r, \tag{3.6}$$

and where $V(|\mathbf{r}_1-\mathbf{r}_2|)=e^2/|\mathbf{r}_1-\mathbf{r}_2|$ is positive definite, it follows that the lowest energy eigenvalue of QHQ is greater than or equal to the sum of the energies of the two lowest hydrogenic levels which conserve the total angular momentum and parity and which have the correct spatial symmetry. The lower bound on $E'_L{}^Q$ obtained in this way for each of the spatial symmetries is given in Table I. If the lowest permissible principal quantum numbers are n_1 and n_2, a lower bound on $E'_L{}^Q$ is given by $-(1-n_1^{-2}-n_2^{-2})E_{T0}$. Since one of the principal quantum numbers is always 2, this reduces to the form $(\frac{3}{4}-1/n^2)$ 13.6 eV.

It follows that at least for $E'<E'_L{}^Q$, η_L for a given symmetry is bounded from below by the phase shift $\eta_L{}^P$ defined by

$$P(H-E)P\Psi_L{}^P=0, \tag{3.7}$$

and by the boundary condition

$$\begin{aligned}\Psi_L{}^P\to{}&\psi_{T0}(\mathbf{r}_1)P_L(\cos\Theta_2)\\&\times\sin(kr_2-\tfrac{1}{2}L\pi+\eta_L{}^P)/r_2\pm(\mathbf{r}_1\to\mathbf{r}_2),\end{aligned} \tag{3.8}$$

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certainly be greater than η^P, by a multiple of π, but one cannot then say how A and A^P compare.

where Θ_2 is the angle between $\mathbf{r}_2$ and a fixed axis. We now point out that the phase shift $\eta_L{}^P$ defined by Eqs. (3.7) and (3.8) is precisely the same as that defined by the usual static approximation. There, one chooses a function of the form

$$\Psi_L{}^P=\psi_{T0}(\mathbf{r}_1)u_0{}^P(\mathbf{r}_2)\pm\psi_{T0}(\mathbf{r}_2)u_0{}^P(\mathbf{r}_1), \qquad (3.9')$$

which satisfies

$$P\Psi_L{}^P=\Psi_L{}^P. \qquad (3.10)$$

(Note that $\Psi_L{}^P$ is *not* equal to $P\Psi_L$.) $u_0{}^P$ is then defined by the integro-differential equation

$$\int\psi_{T0}(\mathbf{r}_1)(H-E)P\Psi_L{}^P(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1=0, \qquad (3.11')$$

or equivalently, by

$$P_1(H-E)P\Psi_L{}^P=0 \qquad (3.12)$$

and by a boundary condition of the form of Eq. (3.8). Interchanging $\mathbf{r}_1$ and $\mathbf{r}_2$, we obtain

$$P_2(H-E)P\Psi_L{}^P=0, \qquad (3.13)$$

from which we, of course, also have that

$$P_1P_2(H-E)P\Psi_L{}^P=0. \qquad (3.14)$$

It follows that

$$P(H-E)P\Psi_L{}^P=0. \qquad (3.15)$$

Since $P_1P=P_1$ (and $P_2P=P_2$), we can also reverse the procedure, going from Eq. (3.15) to Eqs. (3.13) and (3.12). The phase shift as defined by Eqs. (3.7) and (3.8) is then indeed the usual static approximation phase shift.

As for distinguishable particles, the inequality satisfied by η_L and $\eta_L{}^P$ is independent of the choice of the arbitrary multiple of π in the definition of $\eta_L{}^P$.

The lower bound on $E'_L{}^Q$ for electron hydrogen scattering can easily be increased by taking into account to at least some extent the effect of the repulsive e^2/r_{12} term, an effect which has thus far been completely ignored. We will use a technique due to Bazley[11] which is applicable to a Hamiltonian which can be written as H_0+H', where H_0 is solvable and where H' is positive definite. With the choices

$$H_0=Q[H_{\text{hyd}}(\mathbf{r}_1)+H_{\text{hyd}}(\mathbf{r}_2)]Q,$$
$$H'=Q(e^2/r_{12})Q,$$

the theorem is then applicable to the present problem. Though there is no such inherent limitation, we will restrict our considerations to the $L=0$ singlet case. Due to the degeneracy of the $(2s)^2$ and $(2p)^2$ states, one must take at least these two states into account in order to obtain any improvement. We find

$$((2s)^2|(H')^{-1}|(2s)^2)=4.24(-E_{T0})^{-1},$$
$$((2s)^2|(H')^{-1}|(2p)^2)=-0.944(-E_{T0})^{-1},$$
$$((2p)^2|(H')^{-1}|(2p)^2)=3.42(-E_{T0})^{-1},$$

from which we effect the result that the lowest possible energy of QHQ is greater than the smaller of the two numbers 9.6 eV and 8.7 eV, where the 9.6 eV follows from the values obtained from the matrix elements and where the 8.7 eV is the energy associated with one electron in an $n=2$ state and the other in an $n=3$ state. We therefore obtain the improved value of $E'_0{}^Q=8.7$ eV[12] for the $L=0$ singlet case. Further improvement could be obtained by introducing more states, such as the $(2s)$ $(3s)$ and $(2p)$ $(3p)$ states.

The above results may well represent the first self-contained rigorous bounds on a scattering parameter for scattering by a compound system that have ever been obtained, and it is important to understand why this was possible. The bounds on A previously obtained required a knowledge of the number of composite bound states of the target plus incident particle. This number can in principle be obtained theoretically but in practice it has not been and one has had to rely on the experimental evidence. The difficulty with the determination of the number of composite bound states is that there is a continuum of eigenstates of H starting at E_{T0} and we must consider the possibility of bound states of H infinitesimally below E_{T0}. In the present situation, the continuum of QHQ starts at E_{T1} and we need only consider the possibility of bound states of QHQ with energies below E; the gap between E and E_{T1} provides us with the leeway which so greatly increases the possibility of obtaining a rigorous proof.

Lest the above remarks give the wrong impression, it should be noted that very useful results can be obtained even when complete self-consistent rigor is not possible. This point will be emphasized in the paper on minimum principles.

B. Many Fermions, Recoil Negligible

We will now consider problems for which there can be many fermions but for which the recoil effects are negligible, that is, for which there is effectively a center of force. These include the scattering of electrons by atoms and less accurately the scattering of neutrons by heavy nuclei. We will further restrict our considerations to cases for which the target has zero total angular momentum. In this last regard the problem is then slightly simpler than the scattering of electrons by H atoms, for the ground state of the H atom is (spin) degenerate.

Let us discuss the problem in terms of the scattering of an electron by a neutral atom of atomic number Z. It will be convenient here to include the electron spins explicitly. (We did not do so in e^-H scattering.) We expand the fully antisymmetrized scattering function $\Psi(1,\cdots,Z+1)$, in which the numbers represent space

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[11] N. W. Bazley, Phys. Rev. **120**, 144 (1960).

[12] An upper bound of 9.4 eV on the $E'_0{}^Q$ has been obtained in an approximate manner by E. Holøien, Proc. Phys. Soc. (London) **71**, 357 (1958). P. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962), using the $1s+2s+2p$ approximation, have recently found such a resonance in the singlet s-wave phase shift at 9.6 eV.

and spin coordinates, in the form

$$\Psi=\sum_i\{\psi_{Ti}(-[Z+1])u_i(Z+1) - \sum_{k=1}^{Z}\psi_{Ti}(-k)u_i(k)\}, \qquad (3.16)$$

where

$$\psi_{Ti}(-k)=\psi_{Ti}(1,\cdots k-1,k+1,\cdots,Z+1)$$

represents the fully antisymmetrized ith state of the atomic system in which all but the kth electron are present and in which the numbers in the argument are ordered. The $u_i(k)$ are not uniquely defined by Eq. (3.16). Without any loss of generality, the $u_i(k)$ for $i\neq 0$ can be chosen such that

$$(\psi_{T0}(-[Z+1]),\sum_{k=1}^{Z}\psi_{Ti}(-k)u_i(k))=0, \qquad (3.17)$$

where the inner product is over all of the coordinates other than those of the $(Z+1)$th electron, for any component in the sum over k which was not orthogonal to $\psi_{T0}(-[Z+1])$ could have been absorbed into the $\psi_{T0}(-[Z+1])u_0(Z+1)$ term. Defining the projection operator

$$P(-k)=|\psi_{T0}(-k)\rangle\langle\psi_{T0}(-k)|, \qquad (3.18')$$

we then have that

$$P(-[Z+1])\Psi=\psi_{T0}(-[Z+1])u_0(Z+1). \qquad (3.19')$$

If now we define

$$P=\sum_{k=1}^{Z+1}P(-k), \qquad (3.20)$$

we find that

$$P\Psi=\psi_{T0}(-[Z+1])u_0(Z+1) - \sum_{k=1}^{Z}\psi_{T0}(-k)u_0(k). \qquad (3.21')$$

Note that $P^2\Psi=P\Psi$, so that P is indeed a projection operator in the fully antisymmetrized space. We then choose a function Ψ^P of the form

$$\Psi^P=\psi_{T0}(-[Z+1])u_0{}^P(Z+1) - \sum_{k=1}^{Z}\psi_{T0}(-k)u_0{}^P(k), \qquad (3.22)$$

which is then fully antisymmetric and which then satisfies

$$P\Psi^P=\Psi^P, \qquad (3.23)$$

with the $u_0{}^P$ chosen so that

$$P(H-E)P\Psi^P=0, \qquad (3.24)$$

subject to the usual boundary conditions. The phase shift $\eta_L{}^P$ thereby determined is then guaranteed to provide a lower bound on the exact phase shift η_L if $Q(E-H)Q$ can be shown to be a negative definite operator in the space of fully antisymmetrized functions of angular momentum L, where

$$Q=1-P=1-\sum_{k=1}^{Z+1}P(-k) = \sum_i{}'\sum_{k=1}^{Z+1}|\psi_{Ti}(-k)\rangle\langle\psi_{Ti}(-k)|-Z. \qquad (3.26')$$

It would be a simple matter to combine the techniques used in the two fermion cases with a center of force and with a target of total angular momentum $\frac{1}{2}$ and the many fermion case with a center of force and with a target of total angular momentum zero and to thereby generalize the method to be applicable to the many fermion case with a center of force and with a target of total angular momentum $\frac{1}{2}$.

C. The Few-Fermion Problem–Effects of Recoil

Consider the scattering of a neutron of orbital angular momentum L incident on a nucleus of finite mass and of total angular momentum zero. Consider separately the cases for which the total angular momentum of the target plus the incident particle is $L+\frac{1}{2}$ and $L-\frac{1}{2}$. Due to the effects of recoil, the situation is then apparently more complicated than those previously considered, for we have been unable to find the projection operator which directly leads to the static approximation. We can, however, proceed as follows. Feshbach[6] showed that even in the presence of the Pauli principle an equation of the form Eq. (2.26′) could be obtained. An explicit expression of this form was obtained by Coester and Kummel,[13] and, more generally, by Lipperheide.[13] In this explicit expression, the V_{ij} are replaced by U_{ij}, where the U_{ij} can be expressed in terms of the two body potentials and the ground state and excited state wave functions of the target. Having arrived at an equation of the same form as the one that arose in the scattering by a target of a distinguishable particle, we can proceed as in that case. It should be remarked that due to the effects of recoil, the U_{ij} are even more complicated than are the V_{ij}, so that the expression

$$PUQ\frac{1}{Q(E-H)Q}QUP$$

is an extremely formidable one. The applicability of the monotonicity theorem should perhaps be reexamined, but it seems unlikely that any true difficulties should arise. More significantly, it will probably rarely if ever be possible to obtain rigorous bounds on $E'_L{}^Q$. The realization that such a number exists can nevertheless give some insight into the meaning of any numerical results obtained.

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[13] F. Coester and H. Kummel, Nuclear Phys. **9**, 225 (1958); R. Lipperheide, Ann. Phys. (New York) **17**, 114 (1962); H. Feshbach, Ann. Phys. (New York) **19**, 287 (1962).

TABLE II. A list of fairly accurate values of the $L=0$ singlet phase shift for e^-H scattering at $E'=0.6\times13.6$ eV$=8.2$ eV in various approximations. Since E' is less than $E'_0{}^Q$, the phase shift must improve (increase) as one adds more states. The value in the $1s+2s+2p+3d$ approximation is less than that in the $1s+2s+2p$ approximation, but we firmly believe that a more accurate calculation would show this contradiction to be a spurious one. (The values in question are italicized.)

States							
1*s*	2*s*	2*p*	3*s*	3*p*	3*d*		Phase shift
√							0.6704[a]
√	√						0.7115[a]
√		√					0.7040[a]
√	√	√					*0.7707*[a]
√	√	√	√				0.7738[a]
√	√	√		√			0.7770[a]
√	√	√			√		*0.7694*[a]
√	√	√	√	√			0.7814[a]
√	√		√			(all *s* states)	0.75[b]
√	√	√	√	√		(all *s* and all *p* states)	0.88[b]
√	√	√	√	√	√	(all states)	0.894[c]

[a] See reference 5.

[b] Obtained by interpolation of results of C. Schwartz, Phys. Rev. 126, 1015 (1962).

[c] C. Schwartz, Phys. Rev. 124, 1468 (1961).

The procedure of the present subsection could of course also have been applied to the center of force case treated in the previous subsection, but it is clearly preferable when possible to work with the V_{ij} rather than with the U_{ij}.

4. ALLOWANCE FOR SOME VIRTUAL EXCITATION

We now introduce two projection operators, $P^\star$ and $Q^\star$, with the sole requirements that $P^\star$ include P and that $P^\star Q^\star=0$. $P^\star+Q^\star$ need *not* span the entire space. We then define $\Psi^{P^\star}$ and $\Psi^{P^\star+Q^\star}$ as the solutions of

$$P^\star(H-E)P^\star\Psi^{P^\star}=0, \tag{4.1}$$

and

$$(P^\star+Q^\star)(H-E)(P^\star+Q^\star)\Psi^{P^\star+Q^\star}=0, \tag{4.2}$$

respectively, subject to boundary conditions of the usual form, with phase shifts $\eta^{P^\star}$ and $\eta^{P^\star+Q^\star}$. The entire previous discussion then carries over, every numbered equation without primes remaining valid under the replacements $P\rightarrow P^\star$ and $Q\rightarrow Q^\star$. (The terms to be included in $\sum'$, when it appears, must be appropriately modified.) Our final result then is that

$$\eta_L{}^{P^\star+Q^\star}>\eta_L{}^{P^\star} \quad \text{if} \quad Q^\star(E-H)Q^\star<0, \tag{4.3}$$

that is, if the operator is a negative-definite operator. The numerical determination of $\eta^{P^\star}$ is, of course, more difficult than that of η^P since we now have to solve coupled differential (or integro-differential) equations, rather than just one such equation.

A. Electron Hydrogen Scattering

As an example, consider again e^-H scattering. Let

$$P^\star=P_1{}^\star+P_2{}^\star-P_1{}^\star P_2{}^\star, \tag{4.4}$$

where $P_k{}^\star$ contains the projection operators in the space of the kth electron of the 1*s*, 2*s*, and 2*p* states, plus any additional states. The lowest possible state of either electron allowed by $Q^\star$ is then at best the $n=3$ state, so that

$$Q^\star HQ^\star>2\times(1/9)\times(-13.6)\text{ eV}.$$

$Q^\star(E-H)Q^\star$ is then a negative definite operator for E' anywhere from zero right up to $\frac{3}{4}(13.6\text{ eV})=10.2$ eV, that is, right up to the threshold for excitation. It follows that for $0\leq E'<10.2$ eV, one can predict inequalities such as

$$\eta_L>\eta_L{}^{1s+2s+2p+3s}>\eta_L{}^{1s+2s+2p}.$$

Corresponding predictions cannot be made for phase shifts such as those associated with the $1s+2s+2p+3s$ and with the $1s+2s+2p+3p$ approximations. For $E'<E'_L{}^Q$ as given in Table I, we can also be certain of inequalities such as

$$\eta_L>\eta_L{}^{1s+2p}>\eta_L{}^{1s},$$

and

$$\eta_L>\eta_L{}^{\text{all }s}>\eta_L{}^{1s+2s}>\eta_L{}^{1s}.$$

A set of values for the $L=0$ e^-H singlet phase shift, in various approximations, is given in Table II for a typical energy value, $E'=8.2$ eV. The only violation among the 42 predicted inequalities is that η_0 in the $1s+2s+2p+3d$ approximation is less than, rather than greater than, η_0 in the $1s+2s+2p$ approximation. The values differ, however, by only one unit in the third significant figure, the smallest difference between any two listed values; if there is not a fundamental error in the arguments of this paper, it must be true that a more accurate evaluation would remove the discrepancy. (Among other things, the results of the present paper should in this regard be able to serve as a partial check on numerical calculations.) It should, of course, be clear that Burke and Schey were not really concerned about the third significant figure.

B. Positron Hydrogen Scattering

Numerical results have not been obtained in as many approximations for e^+H as for e^-H scattering, but those that have been obtained[5] show the same general character, that is, the phase shift increases on going from $P^\star$ to $P^\star+Q^\star$. This is the predicted behavior *if* there is no discrete state of $Q(H-E_{T0})Q$ in the energy region covered by these calculations, that is, from 0 to 6.8 eV. We have not, however, as in the case of electron scattering, been able to eliminate the possibility of such a state *a priori*, nor have we even been able to obtain a rigorous lower bound on $E'_L{}^Q$. (We might note that the plausible assumption that a positron cannot be bound to a hydrogen atom leads to the conclusion that $Q(H-E_{T0})Q$ is a positive definite operator; this implies in turn that the static approximation scattering length and zero energy phase shift, and therefore the phase shifts up to at least some small energy, provide bounds on the exact quantities.)

Though we will not do so, it should not, however, be at all difficult to examine the reasonability of the prediction that $\eta_L^{P\star+Q\star}$ should be greater than $\eta_L^{P\star}$. Considering the static approximation, for example, one would attempt to find the lowest possible value of $(\Psi_t', H\Psi_t')$, with Ψ_t' having $L=0$ and having the form

$$\Psi_t' = \sum{}' \psi_{Ti}(\mathbf{r}_e) u_i(\mathbf{r}_p),$$

where $\mathbf{r}_e$ and $\mathbf{r}_p$ are the electron and positron coordinates. If with a reasonable effort one could not find a value more than 1 eV for example below $-\frac{1}{2}(13.6) = -6.8$ eV, the bound state of positronium, (which has a lower energy than $E_{T1} = \frac{1}{4}(-13.6)$, the first excited state of the hydrogen atom), one might well believe that there was no value more than say 2 eV below -6.8 eV. It would then follow for $E' < -2-6.8-(-13.6) = 4.8$ eV, that we would have $\eta_0 > \eta_0^{1s}$.

There is one result for e^+H scattering which can be rigorously proved. If we consider only the possibility of s state excitation then the true Hamiltonian

$$H(\mathbf{r}_e,\mathbf{r}_p) = \left(T_e - \frac{e^2}{r_e}\right) + T_p + \frac{e^2}{r_p} - \frac{e^2}{r_{ep}}$$

can be replaced by

$$H^s(\mathbf{r}_e,\mathbf{r}_p) = \left(T_e - \frac{e^2}{r_e}\right) + T_p + \frac{e^2}{r_p} - \frac{e^2}{r_>},$$

where $r_>$ is the larger of r_e and r_p. Since

$$e^2(1/r_p - 1/r_>) \geqq 0,$$

we have that

$$H^s(\mathbf{r}_e,\mathbf{r}_p) \geqq \left(T_e - \frac{e^2}{r_e}\right) + T_p.$$

If one projects out the hydrogenic ground state, it follows that the lowest eigenvalue of H^s is $\frac{1}{4}(-13.6)$ eV, and we have the rigorous result for $0 \leqq E' < 6.8$ eV, the threshold for pickup, that

$$\eta^{\text{all } s} > \cdots > \eta^{1s+2s} > \eta^{1s}.$$

The inequality $\eta^{1s+2s} > \eta^{1s}$ is borne out by the calculations. Note that the above argument does *not* say how any of the s state results compare with the exact phase shift. (Even the all-s state result would not be expected to be particularly accurate, since the virtual formation of positronium is expected to play a significant role.) Since the interaction between the positron and the hydrogen atom that is contained in H^s is repulsive, we also have the inequality $0 > \eta^{\text{all } s}$.

5. POSSIBLE IMPROVEMENTS AND EXTENSIONS

The static approximation can provide a bound, but the bound need not be an accurate one. One can improve the bound by introducing additional states, but the amount of work increases very rapidly and the accuracy of the result will often increase rather slowly. What is needed is a minimum principle in which one can introduce a trial function with an arbitrary number of parameters which are to be varied so as to give the greatest possible value for the phase shift. Such a minimum principle can be obtained by proceeding along the present lines, and it will be presented shortly. It represents an extension of the previous minimum principle,[1,2] which was limited to zero energy. It is a considerable improvement upon the minimum principle previously obtained at nonzero energies[3] for other than potential scattering, since the truncation of potentials and the erection of potential barriers is not required if one solves the static potential problem numerically. The minimum principle is applicable to some multichannel scattering processes, possibly to all.

A very important extension would be to eliminate the requirement that the ground-state wave function be known exactly.

APPENDIX A. ABSOLUTE DEFINITION OF THE PHASE SHIFT

There is one small remark that should be made concerning the absolute definition of the phase shift. The term φ_0 in the expansion, Eq. (3.3), of the spatially antisymmetric but otherwise arbitrary function $\Phi(\mathbf{r}_1,\mathbf{r}_2)$ can be chosen to be orthogonal to ψ_{T0}. (Due to the possibility of a term $\psi_{T0}(\mathbf{r}_1)\psi_{T0}(\mathbf{r}_2)$, this is *not* necessarily so for the spatially symmetric case.) This is true in particular for the triplet scattering function $\Psi(\mathbf{r}_1,\mathbf{r}_2) = -\Psi(\mathbf{r}_2,\mathbf{r}_1)$. The function φ_0 is of course called u_0 for this particular case. We then have that

$$u_0(\mathbf{r}_1) = \int \Psi(\mathbf{r}_1,\mathbf{r}_2)\psi_{T0}(\mathbf{r}_2)d\mathbf{r}_2$$

is orthogonal to $\psi_{T0}(\mathbf{r}_1)$. Since $\psi_{T0}(\mathbf{r}_1)$ is nodeless, $u_0(\mathbf{r}_1)$ must have at least one node, even at zero incident energy. If we define the absolute phase shift for single-channel scattering by a compound system as the phase shift that one would ascribe to potential scattering that would give rise to the scattering function $u_0(\mathbf{r}_1)$, it follows without any detailed analysis that the zero energy phase shift for the triplet scattering of electrons by hydrogen atoms is at least π, a result that has its origins in the workings of the Pauli principle.

This result has been obtained previously.[14] The purpose of the present remarks is only to point out that the absolute definitions given previously are entirely equivalent to defining the phase shift as that associated with one-body scattering by the generalized optical potential. One may thereby be able to utilize results

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[14] See the second paper in reference 3, and A. Temkin, J. Math. Phys. 2, 336 (1961). See also P. Swan, Proc. Roy. Soc. (London) A228, 10 (1955).

obtained, by Martin and others[15] for example, for scattering by nonlocal potentials. It must be recalled, however, that these analyses were concerned with energy-independent nonlocal potentials.

APPENDIX B. CONTINUITY OF THE PHASE SHIFT

We saw in Appendix A that $u_0(\mathbf{r}_1)$ is not uniquely determined if it is defined as the coefficient of $\psi_{T0}(\mathbf{r}_2)$ in the expansion of the triplet scattering wave function. $u_0(\mathbf{r}_1)$ was presumably uniquely defined though, and hence the phase shift was also, if $u_0(\mathbf{r}_1)$ was defined as the solution of the one-body Schrödinger equation with the generalized optical potential, or, equivalently, if it was defined as the inner product of $\psi_{T0}(\mathbf{r}_2)$ with $\Psi(\mathbf{r}_1,\mathbf{r}_2)$. Now in fact there is in general a further assumption that must be made if the phase shift is to be uniquely defined, and if the monotonicity theorem as we have used it is to be valid. This assumption is that the wave function and the phase shift are to be continuous functions of the strength of the potential. (The question only arises under the unlikely circumstances described below.) The assumption is a natural one for our purposes, and is certainly an allowable one, but it is not a necessary one. Though it is not stated so explicitly, a different assumption is used in references 15. There, where one is interested in the difference, $\eta(E=0)-\eta(E=\infty)$, it is natural to assume the phase shift to be a continuous function of the energy. It is there found, for example, for a potential which contains a local potential plus a nonlocal separable potential with strength λ, that as λ increases it can happen that η is greater by π for a particular value λ_0 of λ than it is for neighboring values of λ on either side of λ_0. The monotonicity theorem is not then valid. The difficulty arises because of the presence at $\lambda=\lambda_0$ of a true bound state of energy $E_0>0$, that is, a bound state of infinite lifetime embedded in the continuum. If λ is fixed at λ_0 and the energy is varied, and if the phase shift is taken to be a continuous function of the energy, the wave function will contain some bound state component. If the energy is fixed at E_0 and λ is varied, and if the phase shift is taken to be a continuous function of λ, the wave function will not contain any bound state component as E passes through E_0. With the assumption of continuity in λ, incidentally, Levinson's theorem assumes its usual form, $\eta(E=0)-\eta(E=\infty)=\nu\pi$, where ν is the number of negative energy bound states, there being no contribution to $\eta(E=0)-\eta(E=\infty)$ due to bound states embedded in the continuum as found in reference 15; the effect of the positive energy bound state is to produce a discontinuous jump in η as a function of the energy (the limiting case of an infinitely sharp resonance), rather than a violation of Levinson's theorem.

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[15] M. Gourdin and A. Martin, Nuovo cimento **6**, 757 (1958) and **8**, 699 (1958); A. Martin, *ibid.* **7**, 607 (1958); Kh. Chadan, *ibid.* **10**, 892 (1958).