Low-Energy Scattering by a Compound System: Positrons on Atomic Hydrogen*†‡

LARRY SPRUCH AND LEONARD ROSENBERG
Physics Department, Washington Square College, New York University, New York, New York
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The formalism, developed by Kato, which gives upper and lower bounds on the phase shift for the scattering of a particle by a center of force has been generalized to apply to scattering by a compound system. Particularly simple and useful results are obtained for the case of zero energy scattering where no composite bound state exists. As a first example, because of its relative simplicity, the problem of low-energy positron scattering from atomic hydrogen, with zero total orbital angular momentum, is studied. It is shown that at zero energy the ordinary Kohn variational calculation, which ignores second order contributions, provides an upper bound on the scattering length, from which a bound on the cross section is deduced. For nonzero energies a bound on the phase shift may similarly be obtained, but for a fictitious problem with cutoff potentials. If the energy is sufficiently small (less than 3 ev, say) the error thus incurred is expected to be negligibly small. Numerical calculations performed at $k=0$ and $ka_0=0.2$ lead to the result that at these energies the effects of polarization are large enough to cause the positron to be on the whole *attracted* to the hydrogen atom.

1. INTRODUCTION

IT is somewhat disconcerting that more than thirty years after the advent of quantum theory there exists no general method that may be applied with confidence to the calculation of the cross section for scattering of a particle by a compound system, even if the energy is sufficiently low so that only elastic scattering is possible. The use of a variational method is in itself by no means sufficient to ensure any accuracy whatever. In applications of the Kohn and Hulthén forms of the variational principle certain consistency criteria[1] are frequently used to check the validity of the calculation. It is quite clear, however, that these criteria are by no means completely satisfactory. The knowledge that the consistency ratio is very different from unity is, to be sure, a useful if negative piece of information; the difficulty is that a consistency ratio close to unity may imply nothing more than an accurate calculation within the limitations, however severe and inappropriate, of the assumed form of the wave function. This point has been illustrated by Bransden, Dalgarno, John, and Seaton[2]; a still simpler example of a complete failure of the consistency criteria is found in the present e^+H problem. A trial function involving no polarization of the hydrogen atom will lead to perfect consistency if the positron wave function is the exact solution of the static problem, and yet at low energies we find that polarization plays a crucial role. The weakness of the consistency checks is well recognized, but though all agree with a previous author[3] that "a foolish consistency is the hobgoblin of little minds," these checks have nevertheless been frequently used simply because no better standards have been available.

In the case of scattering by a static central potential, where the cross section, σ, consists of a sum of partial cross sections, σ_L, each of which depends upon just one real number, the phase shift $\bar{\eta}_L$, a number of methods have been devised for determining upper and lower bounds on $\cot\bar{\eta}_L$ and hence on σ_L.[4,5] Perhaps the most general of these methods is the one due to Kato.[5] The method was applied by Kato to the case of $L=0$ with rather striking results. It has also been applied to higher angular momenta[6]; the calculations are then more cumbersome, but useful results can still be obtained. Some improvements in the formalism itself have also been effected, including the minimization of the amount of *a priori* knowledge of $\bar{\eta}_L$ which is required before the method can be applied[7]; this will generally be essential for the compound scatterer where (except for zero energy) one ordinarily has no *a priori* knowledge of $\bar{\eta}_L$ whatever.

It may be noted that the Kato formalism is by no means restricted to quantum mechanical problems; it is applicable to any problem that can be reduced to a set of uncoupled differential equations, each having a solution characterized by a single phase shift. For

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‡ A preliminary report was given at the Washington Meeting of the American Physical Society in April, 1958 [Bull. Am. Phys. Soc. **3**, 171 (1958)].

[1] See, e.g., Yu. N. Demkov and F. P. Shepelenko, J. Exptl. Theoret. Phys. U.S.S.R. **33**, 1483 (1957) [translation: Soviet Phys. JETP **6(33)**, 1144 (1958)]. (These authors, we might note, show that a consistency check and a comparison of the results obtained from the Kohn and Hulthén methods are not independent validity tests.)

[2] Bransden, Dalgarno, John, and Seaton, Proc. Phys. Soc. (London) **71**, 882 (1958).

[3] R. W. Emerson, *Complete Essays* (Random House, New York, 1940), p. 152.

[4] W. Kohn, Revs. Modern Phys. **26**, 292 (1954); T. Kikuta, Progr. Theoret. Phys. (Kyoto) **12**, 225 (1954); **12**, 234 (1954). J. Keller, Nuovo cimento **5**, 1122 (1957); I. C. Percival, Proc. Phys. Soc. (London) **70**, 494 (1957).

[5] T. Kato, Progr. Theoret. Phys. (Kyoto) **6**, 295 (1950); **6**, 394 (1951); Phys. Rev. **80**, 475 (1950).

[6] L. Spruch and M. Kelly, Phys. Rev. **109**, 2144 (1958).

[7] L. Spruch, Phys. Rev. **109**, 2149 (1958).

example, the method has been applied to the study of certain types of electromagnetic waveguides.[8]

It is to be expected that some difficulties will arise in an attempt to generalize the Kato method to scattering by a compound system. These difficulties will be discussed in Sec. 2 where it will also be shown that there exist interesting circumstances under which they can be circumvented. It is further to be anticipated that a calculation which furnishes one or both bounds will be more complicated than a variational calculation. While this is generally the case, there are situations in which an ordinary variational calculation gives a bound.

Of the many-body problems to which the Kato method can be applied we have thought it worthwhile, for reasons of simplicity, to consider first the scattering of positrons by hydrogen atoms.[9,10] (The absence of the Pauli principle and the fact that no three-body bound state exists simplify the analysis.) Of course, the possibility of positron-electron annihilation exists. However, only at extremely small energies will the annihilation process compete with elastic scattering.[11] Our subsequent "zero" energy results (see Sec. 4) may therefore be interpreted as extrapolations from some small nonzero energy.

2. THE KATO METHOD

A. The True Problem

To facilitate subsequent discussion we define a problem with somewhat specialized conditions. We consider the scattering of a particle (particle number 1) of mass m_1 from a system in its ground state consisting of two particles of masses M and m_2, respectively. We take $m_1=m_2\equiv m$ and choose $M\gg m$ so that the scattering system is effectively a particle (particle number 2) of mass m in a field of force. Particles 1 and 2 are assumed to be distinguishable so that we need not concern ourselves with the Pauli principle. Let E_{2g} denote the ground state energy of the second particle in the field of force; ΔE_2 is its minimum excitation energy. Correspondingly, if the first particle can be bound to the center of force, let E_{1g} denote the ground-state energy. If particles 1 and 2 can by themselves form one or more bound states we denote their ground-state energy by E_{12g}. Finally, we let T_1 label the initial kinetic energy of the incident particle. The discussion is limited to scattering states of zero total orbital angular momentum.

The Kato method is applicable only if the scattering problem is such that the various angular momenta are not coupled and if the scattering for a given angular momentum can be completely characterized by one real phase shift. For the scattering of a particle by a center of force, both of these conditions are realized if the potential is spherically symmetric. In the many-body scattering problem we must not only have potentials which are independent of the spatial orientation of the system as a whole, to allow a partial wave analysis, but also certain energy relations must be satisfied if the characterization by one real phase shift is to be possible. In particular, (1) Excitation or ionization must not be possible; i.e., we must have $T_1<\Delta E_2$. (2) Exchange must not be possible, requiring $|E_{2g}|>|E_{1g}|$, and further $T_1<|E_{2g}|-|E_{1g}|$. (3) Pickup must not be possible, requiring $|E_{2g}|>|E_{12g}|$ and further $T_1<|E_{2g}|-|E_{12g}|$.

In the case of positron scattering from hydrogen atoms, we have

$$|E_{2g}|=\tfrac{1}{2}e^2/a_0,\quad \Delta E_2=\tfrac{3}{4}|E_{2g}|,\quad E_{12g}=\tfrac{1}{2}E_{2g}.$$

Exchange is not possible and conditions (1) and (3) above require that T_1 be less than $\frac{3}{4}|E_{2g}|$ and $\frac{1}{2}|E_{2g}|$, respectively. It is necessary therefore that the initial positron energy be less than 6.8 ev in order that one real phase shift completely characterize the $L=0$ scattering.

We return now to the more general problem and assume that conditions (1), (2), and (3) are satisfied. The differential equation to be solved is

$$(2m/\hbar^2)(E-H)\bar{u}_\theta(r_1,r_2,r_{12})/r_1 \equiv(1/r_1)\mathfrak{L}\bar{u}_\theta(r_1,r_2,r_{12})=0, \quad (2.1)$$

where H is the Hamiltonian of the system and $E=E_{2g}+T_1$ is the total energy. Here $r_1=|\mathbf{r}_1|$, $r_2=|\mathbf{r}_2|$, and $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the two particles measured from the center of force. Defining $\epsilon_g=(2m/\hbar^2)|E_{2g}|$, $k^2=(2m/\hbar^2)T_1$, and $W=-(2m/\hbar^2)V$ for all three "potentials" W_1, W_2, and W_{12}, we have

$$\mathfrak{L}=\frac{\partial^2}{\partial r_1^2}+\frac{1}{r_2^2}\frac{\partial}{\partial r_2}r_2^2\frac{\partial}{\partial r_2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\frac{\partial}{\partial p}(1-p^2)\frac{\partial}{\partial p} +W_1(r_1)+W_2(r_2)+W_{12}(r_{12})+k^2-\epsilon_g, \quad (2.2)$$

where p is the cosine of the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$. The exact solution, $\bar{u}_\theta$, must satisfy the boundary conditions

$$\begin{aligned}&\bar{u}_\theta\to\bar{R}(r_2)[\cos(kr_1+\theta)+\cot(\bar{\eta}-\theta)\sin(kr_1+\theta)], \quad \text{as } r_1\to\infty,\\ &\bar{u}_\theta\to 0, \quad \text{as } r_2\to\infty,\\ &\bar{u}_\theta=0, \quad \text{at } r_1=0,\end{aligned} \quad (2.3)$$

where $\bar{R}(r_2)$ is the *exact* ground-state wave function for the bound particle, normalized such that

$$2\int_0^\infty r_2^2 dr_2\bar{R}^2(r_2)=1. \quad (2.4)$$

[8] L. Spruch and R. Bartram (to be published).

[9] H. S. W. Massey and A. H. A. Moussa, Proc. Phys. Soc. (London) **71**, 38 (1958). There is a misprint in Eq. (15) of this paper. See our Eq. (4.14) for the correct version.

[10] H. Moiseiwitsch, Proc. Phys. Soc. (London) **72**, 139 (1958).

[11] W. B. Teutsch and V. W. Hughes, Phys. Rev. **103**, 1266 (1956).

The normalization parameter, θ, satisfies $0\leq\theta<\pi$ but is otherwise arbitrary. The true phase shift, $\bar{\eta}$, is determined by (2.1), (2.2), and (2.3). (We have here, and in the following, dropped the subscript zero on $\bar{\eta}$.)

We now introduce a trial function, $u_\theta(r_1,r_2,r_{12})$, which satisfies the same boundary conditions as $\bar{u}_\theta$ but with the true phase shift, $\bar{\eta}$, replaced by a trial phase shift, η. Note that this still involves the exact wave function, $\bar{R}(r_2)$. The identity

$$k\cot(\bar{\eta}-\theta)=k\cot(\eta-\theta)-\int u_\theta\mathfrak{L}u_\theta d\tau+\int w_\theta\mathfrak{L}w_\theta d\tau \quad (2.5)$$

then carries over from the one-body case where now $d\tau=dr_1r_2^2dr_2dp$ and where

$$w_\theta(r_1,r_2,r_{12})=u_\theta(r_1,r_2,r_{12})-\bar{u}_\theta(r_1,r_2,r_{12}). \quad (2.6)$$

Since w_θ is a first order term, Eq. (2.5) constitutes a variational principle for $\cot(\bar{\eta}-\theta)$ upon dropping the last term.

B. The Associated Eigenvalue Problem

Consider the equation

$$\mathfrak{L}\phi-\mu\rho\phi=0, \quad (2.7)$$

where ρ is a non-negative function to be chosen such that the scattering problem determined by Eq. (2.7) and by appropriate boundary conditions is characterized for each value of μ by one real phase shift, $\delta(\mu)$. Then there exists an infinite set of discrete eigenvalues $\mu_{n,\theta}$ and corresponding eigenfunctions $\phi_{n,\theta}$ normalized by

$$k^{-1}\int\phi_{n,\theta}\phi_{m,\theta}\rho d\tau=\delta_{nm},\quad m,n=0,\pm1,\pm2,\cdots, \quad (2.8)$$

where δ_{nm} is the Kronecker δ-symbol, such that

$$\begin{aligned}&\phi_{n,\theta}\to\text{const}\bar{R}(r_2)\sin(kr_1+\theta+n\pi),\quad\text{as}\quad r_1\to\infty,\\&\phi_{n,\theta}\to0,\quad\text{as}\quad r_2\to\infty,\\&\phi_{n,\theta}=0,\quad\text{for}\quad r_1=0.\end{aligned} \quad (2.9)$$

We denote the smallest positive eigenvalue of the set $\mu_{n,\theta}$ by α_θ and the smallest (in magnitude) negative eigenvalue by $-\beta_\theta$. The Kato inequalities are

$$-\alpha_\theta^{-1}\int(\mathfrak{L}u_\theta)^2\rho^{-1}d\tau\leq\int w_\theta\mathfrak{L}w_\theta d\tau\leq\beta_\theta^{-1}\int(\mathfrak{L}u_\theta)^2\rho^{-1}d\tau. \quad (2.10)$$

This formal development follows that for the one-body problem, *mutatis mutandis*. However, the actual restrictions on ρ, referred to above, involve considerations peculiar to the many-body problem. We observe first a restriction which does carry over from the one-body case, namely, that ρ must vanish faster than $1/r_1$ as r_1 becomes infinite in order that normalization according to Eq. (2.8) be possible and the phase shift, $\delta(\mu)$, be defined. The choice $\rho=\rho(r_2)$, for example, is eliminated.[12] To eliminate pickup in the associated eigenvalue problem, which is defined for an infinitely broad range of potential strengths, there are two alternatives.

(a) Choose ρ to be independent of r_{12}, at least for r_1 and/or $r_2\to\infty$. Then E_{12g} will be independent of μ.

(b) Imagine the bound particle to be enclosed in a box with perfectly rigid walls. The size of the box, although finite, may be large enough so that the deviation of the phase shift from that for the *real* problem is negligibly small.

The exchange process may occur in the associated problem even if it is absent in the real problem. Again there are two alternative solutions.

(a′) Choose ρ to be independent of r_1, at least for $r_2\to\infty$. Then E_{1g} will be independent of μ.

(b′) Put the bound particle in a box, as in (b) above.

If this latter suggestion is adopted we require

$$r_1\rho(r_1,r_2,r_{12})\to0,\quad\text{as}\quad r_1\to\infty, \quad (2.11)$$

but ρ is otherwise arbitrary.

3. APPLICATION TO POSITRON SCATTERING BY HYDROGEN

Kato has shown for the static central potential that if the potential cuts off outside a region of radius a then $\beta_\theta=\infty$ if, in addition, the following conditions are satisfied:

(1) $ka<\pi-\theta$,

(2) $\bar{\eta}<\theta<\pi$.

This is a particularly interesting case since then a lower bound may be obtained on the phase shift without the necessity of evaluating the more difficult integral, $\int(\mathfrak{L}u_\theta)^2\rho^{-1}d\tau$. The analogous result holds in the three body problem considered in Sec. 2. [In this case the required proof that $\delta(-\infty)=-ka$ (where $\rho=0$ for $r_1>a$) is slightly more involved, though still trivial.[13]]

The many-body problem is generally complicated by the difficulty that one cannot get even crude bounds on $\bar{\eta}$, so that condition (2) cannot be proved (assuming that it is true). We have recourse here to the use of a

[12] The theorem which states that the phase shift for scattering by a center of force is a monotonic function of the potential strength for a potential of constant sign carries over to the many-body case *provided* that the unperturbed energy of the compound system remains fixed as the potential strength varies. Thus, another reason for demanding that ρ vanish with large r_1 is that the required monotonicity of $\delta(\mu)$ with μ will not be preserved if ρ becomes some function of r_2 as $r_1\to\infty$. Furthermore, for large negative values of μ, particle 2 would no longer be bound. The boundary conditions, Eq. (2.9), would then be violated.

[13] See L. Spruch and L. Rosenberg, Research Report No. CX-40, Division of Electromagnetic Research, Institute of Mathematical Sciences, New York University (unpublished).

"conditional inequality."[7] We simply *assume* that condition (2) is satisfied; the subsequent "conditional inequality" for $k\cot(\bar{\eta}-\theta)$ may or may not be valid. However, the bound on $\bar{\eta}$ deduced from the "conditional inequality" on $k\cot(\bar{\eta}-\theta)$ will be valid *whether or not* the bound on $k\cot(\bar{\eta}-\theta)$ is valid, and therefore *whether or not* condition (2) is in fact satisfied.

Turning to the e^+H problem, we consider the set of "potentials"

$$W_1(r_1)+W_{12}(r_{12})=-2(a_0r_1)^{-1}+2(a_0r_{12})^{-1}, \quad r_1\leq a, \qquad =0, \quad r_1>a, \tag{3.1}$$

where a_0 is the Bohr radius. For k sufficiently small, a may be chosen large enough so that the neglect of the true positron-hydrogen interaction which exists beyond $r_1=a$ introduces a negligible error in the phase shift. If k is zero, we may let a become infinite, in which case no distortion of the true potentials is introduced.[14] In this case, the validity of the second condition stated above, namely $\bar{\eta}<\theta<\pi$, is deduced by assuming that no three-body bound state exists for the positron-hydrogen system (none has been found either experimentally or theoretically[15]). We then apply a theorem which is the generalization to many-body systems of a theorem proved by Levinson[16] for the scattering from a static potential. It states that when the exclusion principle is not in effect the phase shift for zero energy scattering is $n\pi$ where n is the number of bound states of the composite system.[17,18] From this we conclude that $\bar{\eta}=0$ for $k=0$. A completely rigorous proof of the above theorem has not been given even for potentials which fall off rapidly. A proof for the slowly decaying Coulomb forces will be even more difficult, although the result (assuming it applies to rapidly decaying potentials) is perhaps made more reasonable by the observation that the "effective interaction" of the positron or electron with the atomic system falls off fairly rapidly. For e^+ on H, e.g., it goes as $1/r^4$. Actually, as will be noted in Sec. 5, the numerical results we have obtained for the e^+H problem do not depend on the validity of the above-mentioned theorem.

[14] Actually, as discussed in Sec. 2, the electron is to be thought of as enclosed in a large box, which has no effect on the true problem at zero energy but which limits the number of allowable processes which can take place in the associated problem.

[15] C. Frönsdal and A. Ore, Physica **19**, 605 (1953).

[16] N. Levinson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **25**, No. 9 (1949). See also, J. M. Jauch, Helv. Phys. Acta **30**, 143 (1957); and J. C. Polkinghorne, Proc. Cambridge Phil. Soc. **54**, 560 (1958).

[17] R. Newton, Ann. Phys. **4**, No. 1, 29 (1958).

[18] A generalization of Levinson's theorem to scattering by a compound system has been given by Swan [P. Swan, Proc. Roy. Soc. (London) **A228**, 10 (1955)], including the effects of the exclusion principle, subject however to the approximation that the polarization of the compound system can be neglected. (We might note that in the absence of the Pauli principle the static approximation leads directly to the usual differential equation for which Levinson's theorem is known to be true.) By virtue of the profound effects of polarization in the present problem (see Sec. 4), results based on the static approximation clearly have no relevance here.

With the choice $\theta=\frac{1}{2}\pi$ and with the definitions

$$-\bar{A}\equiv\lim_{k\to 0}\bar{\eta}/k, \quad -A\equiv\lim_{k\to 0}\eta/k,$$

$$\hat{u}\equiv\lim_{k\to 0}u_{\frac{1}{2}\pi}/k,$$

we have the following bound on the scattering length, $\bar{A}$:

$$\bar{A}\leq A-\int \hat{u}\mathfrak{L}\hat{u}d\tau, \tag{3.2}$$

where $\hat{u}$ has the asymptotic form

$$\hat{u}\underset{r_1\to\infty}{\longrightarrow}\hat{u}_\infty\equiv(2/a_0^3)^{\frac{1}{2}}e^{-r_2/a_0}(A-r_1). \tag{3.3}$$

One of the strong features of the Kato method is that in general it provides a different bound for each choice of θ. This is not true at $k=0$, however, where the identical result is obtained for any θ other than $\theta=0$. The choice $\theta=0$ will lead to a valid bound on $\bar{A}$ only if $\bar{\eta}$ approaches zero from below as k goes to zero, i.e., only if $\bar{A}$ is positive. In this case we have

$$\bar{A}^{-1}\geq A^{-1}+A^{-2}\int \hat{u}\mathfrak{L}\hat{u}d\tau. \tag{3.4}$$

If $\hat{u}$ is sufficiently close to the true function such that A is positive and such that $|\hat{I}|\ll A$, where

$$\hat{I}\equiv\int \hat{u}\mathfrak{L}\hat{u}d\tau,$$

then Eq. (3.4) may be rewritten as

$$\bar{A}\leq A-\hat{I}+A^{-1}\hat{I}^2+\cdots, \quad |\hat{I}|\ll A. \tag{3.4'}$$

It then follows (since $A>0$) that Eq. (3.2) is superior to Eq. (3.4). Therefore, for the special case of zero energy scattering, where no composite bound state exists, the problem of the optimum choice of θ is particularly simple. One should use Eq. (3.2), which follows from any choice of θ satisfying $0<\theta<\pi$.

4. NUMERICAL CALCULATION

A. No Polarization Approximation, $k=0$

To begin with, we consider the class of trial functions of the form

$$\hat{u}(r_1,r_2,r_{12})=g(r_2)f(r_1). \tag{4.1}$$

The required asymptotic form fixes $g(r_2)$ as

$$g(r_2)=\bar{R}(r_2)=(2/a_0^3)^{\frac{1}{2}}e^{-r_2/a_0}.$$

We also have

$$f(0)=0, \qquad f(r_1)\longrightarrow A-r_1, \quad \text{as} \quad r_1\longrightarrow\infty. \tag{4.2}$$

A trial function in this product form corresponds to the approximation (variously referred to as the no polarization approximation, the static approximation, and the one-body approximation) in which the hydrogen atom is not polarized by the incoming positron. We substitute the above expression for $\hat{u}$ into Eq. (3.2) and integrate over r_2 and p. Dropping the subscript on r_1 we find

$$\bar{A}\leq A-\int_0^\infty f(r)\mathfrak{L}_s f(r)dr, \tag{4.3}$$

where

$$\mathfrak{L}_s=d^2/dr^2+W_s(r), \tag{4.4}$$

and

$$W_s(r)=-(2/a_0)e^{-2r/a_0}(1/a_0+1/r), \tag{4.5}$$

so that in the static approximation the positron is repelled by the hydrogen atom. The best possible choice for $f(r)$ would be $f_s(r)$, the exact wave function for scattering by a fixed potential, $W_s(r)$. This will now be shown to follow from an application of the Kato method to this one-body problem.[19] Since no bound state exists for the potential $W_s(r)+\mu\rho(r)$ with μ negative we conclude from Levinson's theorem that

$$\delta(\mu)=0, \quad \mu<0, \tag{4.6}$$

and therefore that $\beta_{\frac{1}{2}\pi}=\infty$. Thus, for any trial function, $f(r)$, we have

$$\bar{A}_s\leq A-\int_0^\infty f(r)\mathfrak{L}_s f(r)dr, \tag{4.7}$$

where $\bar{A}_s$ is the exact scattering length for the static problem. Since the equality holds only when $f(r)=\bar{f}_s(r)$, the statement above has been verified. From Eq. (4.3) with $f(r)=\bar{f}_s(r)$ we find that

$$\bar{A}\leq\bar{A}_s. \tag{4.8}$$

In point of fact one cannot solve for $\bar{f}_s(r)$. However, since we are dealing here with the scattering by a static potential, at zero angular momentum and zero energy, it is a trivial matter to find an upper bound on $\bar{A}_s$ and hence on $\bar{A}$. We will also find a lower bound on $\bar{A}_s$; a comparison of this lower bound with the upper bound we shall subsequently deduce, taking into account the effects of polarization, will give a measure of the limit to the accuracy of the static approximation.

We have already shown that $\beta_{\frac{1}{2}\pi}=\infty$. Choosing $\rho(r)=-W_s(r)$ we observe that $\alpha_{\frac{1}{2}\pi}$ is the smallest positive value of μ for which the "potential" $W_s(r)(1-\mu)$ can support a bound state, for the appearance of a bound state indicates that the phase shift has jumped from zero to π. [Actually, $\delta(\alpha_{\frac{1}{2}\pi})=\frac{1}{2}\pi$.] Since $W_s(r)\times(1-\mu)$ isn't even attractive until $\mu=1$, we immediately obtain $\alpha_{\frac{1}{2}\pi}>1$. This lower bound can be improved quite easily. Bargmann[20] has shown that a necessary condition for the existence of a bound state for a "potential" $U(r)$ is

$$\int_0^\infty r|U(r)|dr\geq 1. \tag{4.9}$$

With $U(r)=-(1-\mu)W_s(r)$, this leads to $\alpha_{\frac{1}{2}\pi}>5/3$.[21] If we choose

$$f(r)=A(1-e^{-nr/a_0})-r(1+Be^{-qr/a_0}) \tag{4.10}$$

we find, with $n=1.5$ and $q=2$, that

$$0.5762a_0\leq\bar{A}_s\leq 0.5823a_0. \tag{4.11}$$

At the same time we have

$$\bar{A}\leq 0.5823a_0. \tag{4.12}$$

The cross section at zero energy, $\sigma(k=0)$, is $4\pi A^2$. The above result without an accompanying lower bound does not exclude a large negative value of $\bar{A}$ and therefore does not provide an upper *or* lower bound on $\sigma(k=0)$.

It is interesting to note that a lower bound on $\bar{A}_s$ has also been determined (though with less accuracy), without performing a variational calculation.[13]

B. Polarization Considered, $k=0$

A trial function of the form $\hat{u}=g(r_1,r_2)$ may take into account, to some extent, the polarization of the hydrogen atom. It may be shown,[13] however, using arguments quite similar to those employed in subsection 4A, that this type of trial function leads to a positive bound on the scattering length, a conclusion which is independent of the particular form of $g(r_1,r_2)$.

It is clear that a realistic trial function should depend on r_1, r_2, *and* r_{12}. This dependence was chosen under the physically plausible assumption that the polarization is largely accounted for by the virtual formation of positronium. Since the latter has a ground-state function proportional to $\exp(-\frac{1}{2}r_{12}/a_0)$, the term $C\exp[-(tr_{12}/a_0)-(vr_2/a_0)]$, the additional factor being required for convergence, was added to a function similar in form to the trial function, Eq. (4.10), which was so successful in the static calculation. We have chosen

$$\begin{aligned}\hat{u}(r_1,r_2,r_{12})=(2/a_0^3)^{\frac{1}{2}}[&Ae^{-r_2/a_0}(1-e^{-r_1/a_0})\\&-r_1e^{-r_2/a_0}+Br_1e^{-(qr_1/a_0)-(sr_2/a_0)}\\&+Cr_1e^{-(tr_{12}/a_0)-(vr_2/a_0)}].\end{aligned} \tag{4.13}$$

The presence of excited states of positronium would spread out the wave function and one would therefore expect that a value of t slightly less than $\frac{1}{2}$ would be the

[19] It should be emphasized that in the remainder of subsection A various quantities, and in particular, β_θ and α_θ, refer to this (static) one-body problem and not to the true problem.

[20] V. Bargmann, Proc. Natl. Acad. Sci. U.S. 38, 961 (1952).

[21] A comparison of $(1-\mu)W_s(r)$ with the Hulthén potential (see the second paper mentioned in reference 5) leads to $\alpha_{\frac{1}{2}\pi}>2$. We prefer, however, to base the present result on an application of the Bargmann theorem rather than on this rare occurrence of an excellent comparison potential for which solutions may be obtained analytically.

TABLE I. Results for $k=0$, with the trial function given by Eqs. (4.13) and (4.15), corresponding to the set of exponential parameters $\{q, s, t, v\}=\{0.50, 0.95, 0.46, 0.78\}$. The consistency ratio, R_K is defined as $R_K=(A-\int \hat{u}\mathfrak{L}\hat{u}d\tau)/A$. The second calculation ($D\neq 0$) yielded a trial function containing no nodes. Note that while the second result is an improvement over the first, its consistency ratio deviates further from unity.

A/a_0	B	C	D	Upper bound on $\bar{A}/a_0$	Lower bound on $\sigma(k=0)$	R_K
−1.3714	2.6516	−1.4620	0	−1.356	$7.357\pi a_0^2$	0.989
−1.4453	2.8106	−1.4979	−0.0532	−1.397	$7.802\pi a_0^2$	0.966

best choice. A number of sets of values of the exponential parameters q, s, t, and v were tried, but nothing even approaching a systematic determination of the best set was attempted. "Best" is here defined as the set which gives the lowest upper bound on $\bar{A}$. Since the results were found to be quite sensitive to the choice of the exponential parameters the realization that $\bar{A}$ satisfies a minimum principle was a great computational advantage. The linear parameters were of course determined variationally for each choice of the exponential parameters. Results are given in Table I.[22]

The effect of polarization is rather dramatic. The value of $\bar{A}$ is negative so that, contrary to the situation in the static approximation, the positron is on the whole *attracted* to the hydrogen atom. Further, an upper bound on $\bar{A}$ now yields a lower bound on $\sigma(k=0)$.

We note incidentally that the best value of t among the sets considered was $t=0.46$, i.e., somewhat smaller than $\frac{1}{2}$, as expected.

Massey and Moussa[9] used a trial function of the form

$$u(r_1,r_2,r_{12})=(2/a_0^3)^{\frac{1}{2}}e^{-r_2/a_0}\times\{\sin kr_1+[a+(b+cr_{12})e^{-r_1/a_0}\times(1-e^{-r_1/a_0})]\cos kr_1\}. \quad (4.14)$$

They determined $\bar{\eta}$ variationally for various values of k, the smallest of which was $k=0.2/a_0$. Presumably they avoided $k=0$ because they did not trust the form of their trial function for that value of k. If, nevertheless, we use their form we find $\bar{A}\approx 0.512a_0$; this value does not differ appreciably from that obtained under the static approximation. It should be noted that despite the extremely poor value for $\bar{A}$ the above calculation provides a consistency ratio

$$R_K=\left(A-\int \hat{u}\mathfrak{L}\hat{u}d\tau\right)\Big/A=1.04.$$

It is rather surprising that the two trial functions, Eqs. (4.13) and (4.14), each containing r_{12} dependence and *three* variational parameters, lead to such strikingly different results, corresponding as they do to an effective attraction in one case and to an effective repulsion in the other. These results speak strongly for the need for obtaining bounds.

It would be difficult to say how reliable our result is without obtaining a *lower* bound on $\bar{A}$. We have been unable to do so, for we have been unable to obtain a lower bound on α_θ. (The difficulty is connected with our inability to prove formally that a composite bound state for $e^+ + H$ does not exist.) We therefore sought additional criteria for the accuracy of our results.

In particular, since no composite bound state exists, we expect by analogy with the one-body problem that $\hat{u}$ should be nodeless. The trial function given by Eq. (4.13) has nodes, although at physically uninteresting points (r_2 large). Since attempts to remedy this by varying the exponential parameters were unsuccessful another term was added. This term was taken to be proportional to $\exp(-\delta r_{12}/a_0)$; if one thinks of this term as being related to the virtual formation of positronium in its first excited state (it does not have precisely the correct form), one might expect that δ should be somewhere near $\frac{1}{4}$. Further, since our previous exponential factors directly coupled r_2 and r_1, and r_2 and r_{12}, we have in this case chosen the additional term to couple r_1 and r_{12}. We take it to be proportional to $\exp(-2r_1/a_0)$. The final form is

$$\hat{u}(r_1,r_2,r_{12})=\hat{u}\,[\text{Eq. (4.13)}]+(2/a_0^3)^{\frac{1}{2}}Dr_1e^{-r_{12}/4a_0-2r_1/a_0}. \quad (4.15)$$

The results are collected in Table I.

The linear parameters were determined variationally, i.e., without regard to the question of nodes; the resultant trial function is nevertheless nodeless. Further, the bound on $\bar{A}$ was lowered only slightly. These two results suggest (in the absence of the other bound on $\bar{A}$ we do not use a stronger word) that our bound on σ may well be reasonably close to the true value. On the other hand our trial function does not indicate the presence of an effective polarization potential which falls off asymptotically like $1/r^4$, as demanded by perturbation theory.[2]

Our trial function, Eq. (4.15), may now be used to estimate the effective range,[23] r_0, for the e^+H system, from the relation

$$r_0=(2/A^2)\int(\hat{u}_\infty^2-\hat{u}^2)d\tau. \quad (4.16)$$

The asymptotic function, $\hat{u}_\infty$, is defined by Eq. (3.3). We find

$$r_0\approx 11a_0. \quad (4.17)$$

This very large value of the effective range severely restricts the domain of applicability of the shape independent approximation,

$$k\cot\bar{\eta}\approx -\bar{A}^{-1}+\tfrac{1}{2}k^2r_0. \quad (4.18)$$

[22] The integrals required in this and subsequent calculations are evaluated in reference 13.

[23] J. M. Blatt and J. D. Jackson, Phys. Rev. **76**, 18 (1949); H. A. Bethe, Phys. Rev. **76**, 38 (1949).

At the very best (if the coefficient of $k^4r_0^3$ in the next term is small[23] and if the expansion is in fact of the same form as for the one-body case[24]) Eq. (4.18) should be useful only for kr_0 somewhat less than unity, i.e., ka_0 somewhat less than 0.1.

C. Polarization Considered, $k\neq 0$

As indicated in Sec. 3, a bound on the phase shift may be obtained for $k\neq 0$ provided a cutoff potential is introduced; for sufficiently small nonzero energies the cutoff point may be made large enough so that the difference between $\bar{\eta}$ and $\bar{\eta}_c$ (the phase shift in the presence of the cutoff potentials) is negligibly small. To illustrate the procedure we describe here a determination of a lower bound on $\bar{\eta}_c$ for $ka_0=0.2$.

To begin with we ignore the question of obtaining a bound and perform an ordinary variational calculation for the true problem. We use a trial function which reduces, as $k\rightarrow 0$, to the zero energy function, Eq. (4.15), namely,

$$u_{\frac{1}{2}\pi}(r_1,r_2,r_{12})/k=(2/a_0^3)^{\frac{1}{2}}[Ae^{-r_2/a_0}\cos kr_1(1-e^{-r_1/a_0}) -e^{-r_2/a_0}\sin kr_1/k+Br_1e^{-qr_1/a_0-sr_2/a_0} +Cr_1e^{-(tr_{12}/a_0)-(vr_2/a_0)}+Dr_1e^{-(r_{12}/4a_0)-(2r_1/a_0)}]. \quad (4.19)$$

(The exponential parameters are fixed at the values cited in Table I.) From the asymptotic form of this function we see that $A=-\tan\eta/k$. The variational principle is now

$$k\tan\bar{\eta}\approx k\tan\eta+\int u_{\frac{1}{2}\pi}\mathfrak{L}u_{\frac{1}{2}\pi}d\tau, \quad (4.20)$$

where $\mathfrak{L}$ is given by Eq. (2.2). The result of the calculation is $\eta=0.1645$,

$$I=\int u_{\frac{1}{2}\pi}\mathfrak{L}u_{\frac{1}{2}\pi}d\tau=-0.0017/a_0,$$

and $\bar{\eta}\approx 0.156$. As a point of comparison we note that a variational calculation (including polarization) performed by Massey and Moussa[9] for the same scattering energy gave $\bar{\eta}\approx -0.098$.

Since the trial function is based on the zero energy function which we expect to be quite good, we have obtained what we believe to be an accurate estimate of $\bar{\eta}$, although not necessarily a lower bound. Before considering the calculation involving the cutoff potentials we recall that the cutoff point, a, is limited by the condition $ka<\pi-\theta$. In order to be able to pick the largest value of a (for fixed k) we wish to choose the smallest value of θ consistent with the condition $\bar{\eta}<\theta$. (Note that we desire that this relation be satisfied, in order that our bound be a *useful* one. As discussed previously, the bound will be *valid* in either case.) The trial function, Eq. (4.19), is normalized with $\theta=\frac{1}{2}\pi$. This would lead to $a=7.9a_0$. In order to obtain a variational estimate of $\bar{\eta}$ corresponding to the use of a trial function with different (and smaller) θ-normalization, we may simply choose

$$u_\theta=u_{\frac{1}{2}\pi}\cos\eta/\sin(\eta-\theta), \quad (4.21)$$

so that

$$k\cot(\bar{\eta}-\theta)\approx k\cot(\eta-\theta)-[\cos\eta/\sin(\eta-\theta)]^2I, \quad (4.22)$$

where η and I have already been determined. We expect that this variational estimate of $\bar{\eta}$ should change very slowly as θ is decreased from $\frac{1}{2}\pi$. It is found, in fact, that to three significant figures the result is unchanged for θ as small as 0.34. (Smaller values of θ lead to appreciably lower estimates of $\bar{\eta}$.) We have therefore chosen $\theta=0.3400$ which allows us to pick $a=14a_0$.

To obtain a bound on $\bar{\eta}_c$ we must now perform a similar calculation with $\mathfrak{L}$ replaced by $\mathfrak{L}_c$ which contains the cutoff potentials, Eq. (3.1). The trial function, $u_{\theta,c}$, must now satisfy the additional requirement that $\mathfrak{L}_cu_{\theta,c}=0$ for $r_1>a$[25], while $u_{\theta,c}$ must of course be continuous in slope and value. It may be shown[13] that a function, $u_{\theta,c}$, may be chosen such that, with $a=14a_0$,

$$\int u_{\theta,c}\mathfrak{L}_cu_{\theta,c}d\tau-\int u_\theta\mathfrak{L}u_\theta d\tau$$

is negligibly small. Therefore, the variational estimate of $\bar{\eta}$ is actually a bound on $\bar{\eta}_c$ and hence is extremely likely to be a bound on $\bar{\eta}$ itself, since the contribution of the potential in the region $r_1>a$ is expected to be extremely small. Results appear in Table II.

TABLE II. Results for $ka_0=0.2$, using a trial function, $u_{\theta,c}$, which is a slight modification of the function given in Eq. (4.19). [The exponential parameters in Eq. (4.19) were taken to be the same as those cited in Table I.] The bound is obtained on $\bar{\eta}_c$, the $L=0$ phase shift for the problem in which the positron interaction vanishes outside a sphere of radius $14a_0$. Thus the difference between $\bar{\eta}$ and $\bar{\eta}_c$ is extremely small. A previous variational calculation,[a] for the same energy, gave $\bar{\eta}\approx -0.098$. All phase shifts are in radians.

A/a_0	B	C	D	Lower bound on $\bar{\eta}_c$
−0.8285	2.0434	−1.1271	0	0.150
−0.8300	2.1159	−1.1464	−0.0412	0.156

[a] See reference 9.

It is easily shown, in the one-body problem, that if the potential vanishes beyond $r=a$, and further, if $ka+\bar{\eta}<\pi$, then the wave function is nodeless in the region $r<a$. Thus, the standard definition of the phase shift, i.e.,

$$\bar{\eta}=\lim_{n\rightarrow\infty}(n\pi-k\rho_n), \quad (4.23)$$

[24] In the e^+H or e^-H problem, for example, $\bar{\eta}_L$ does *not* vanish with k like k^{2L+1} for $L>0$ (due to the long-range polarization potential). Here the effective-range theory, in its usual form, would not be applicable. (See reference 2.)

[25] This may be seen from the fact that in order to obtain $\beta_\theta=\infty$, ρ must vanish beyond $r_1=a$. However, $\int(\mathfrak{L}u_{\theta,c})^2\rho^{-1}d\tau$ should exist.

can be written, in this case, as

$$\bar{\eta}=n\pi-k\rho_n, \quad \rho_n\geq a, \tag{4.23'}$$

where ρ_n is the nth zero (not including the zero at the origin) in the wave function. Now consider the point $r'=(\pi-\bar{\eta})/k$. From the assumed restriction on $\bar{\eta}$ it is clear that $r'>a$. Now the wave function takes on its asymptotic form beyond the point a, and must therefore vanish at r'. But from Eq. (4.23'), $r'=\rho_1$, so that we have shown that the first zero occurs beyond a. In the present problem, under similar conditions (i.e., $W_1+W_{12}=0$ for $r_1>a$, and $ka+\bar{\eta}<\pi$) it may be shown that the function

$$g(r_1)\equiv\int\int r_2^2 dr_2 dp \bar{R}(r_2)\bar{u}(r_1,r_2,p) \tag{4.24}$$

is nodeless for $r_1<a$. For a large enough it seems reasonable (we have not proved it) that a stronger statement can be made, namely, that $\bar{u}$ itself is nodeless for $r_1<a$. If we assume this statement to be true, it may be used to test our trial function. With $D=0$ the function has nodes for $r_1<a$ but these nodes do in fact disappear when the full trial function is used. Further, this improvement in the trial function is accompanied by only a small improvement in the bound on the phase shift. Both of these considerations suggest that this bound may well be in the neighborhood of the true value.

5. DISCUSSION

In our application of the Kato method to the case of zero energy e^+H scattering we have made use of two assumptions, the completeness of the set of solutions, $\phi_{n,\theta}$, of the associated eigenvalue equation (Sec. 2), and the validity of the generalization of Levinson's theorem to scattering by a compound system (Sec. 3). The derivation of the inequality for the scattering length, as we have presented it here, will then be completely justified only when the validity of the above two assumptions has been rigorously established.

We wish to point out, however, that the upper bound deduced for the e^+H scattering length is rigorous. It will be observed that the final result, the expression for the bound, contains no reference to the associated eigenvalue problem. This suggests that the final result, if true, can be derived in a simpler, more direct fashion, independently of the Kato method. This has in fact turned out to be the case, and the proof has been given for far more complicated systems than that considered here.[26] Further, an extension of this result has been obtained to include situations where bound states do exist.[27] These latter methods, however, are limited to the case of zero energy scattering and are specifically designed to provide only the upper bound. Since the Kato method is in principle applicable at *all* scattering energies and can provide *both* bounds on the phase shift we believe it to be well worth further investigation, notwithstanding the various mathematical difficulties which we have encountered, and it is for that reason that we have presented in this paper the Kato method as generalized to scattering of a particle by a compound system.

We might note that for scattering by a center of force for which there is no bound state, the fact that the Kohn variational principle gives an upper bound on the scattering length follows rigorously from the Kato formalism, for in this case there is no question as to completeness or as to the validity of Levinson's theorem.

The bound obtained on the e^+H phase shift for $k\neq 0$ has not received independent justification in the present paper. (It can be done; we hope to return to this point in the future.) However, even as a variational calculation the result is noteworthy; we believe that the trial function used was an extremely accurate one since it was taken to be a direct extension of the zero energy function constructed with the aid of a rigorous minimum principle.

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APPENDIX

The boundary conditions chosen for the eigenfunctions, $\phi_{n,\theta}$, i.e., Eqs. (2.9), are the most straightforward generalization to the many-body problem of the form used originally by Kato for the scattering of a particle by a center of force, namely,

$$\begin{aligned}&\phi_{n,\theta}(r)\rightarrow \text{const}\sin(kr+\theta+n\pi),\\ &\phi_{n,\theta}(0)=0.\end{aligned} \tag{A.1}$$

It is, however, more reasonable to assume that in order to obtain a complete set of eigenfunctions the operator $\mathfrak{L}+\mu\rho$ should be Hermitian, i.e., the boundary conditions should be taken as[28]

$$\int w\mathfrak{L}\phi_{n,\theta}d\tau-\int \phi_{n,\theta}\mathfrak{L}w d\tau=0. \tag{A.2}$$

[26] L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960); Proceedings of the International Conference on Nuclear Forces and the Few Nucleon Problem, London, July, 1959 [Pergamon Press, New York (to be published)].

[27] Rosenberg, Spruch, and O'Malley, Phys. Rev. (to be published).

[28] We shall not attempt to give a proof of completeness under the assumption of Eqs. (2.7) and (A.2). For a rather general though not entirely rigorous proof of the completeness of eigenfunctions of a positive-definite, Hermitian operator see P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 777.

The equivalence between Eq. (A.1) and the one-body form of Eq. (A.2) may easily be displayed. This equivalence does not carry over to the present problem, however. If there exist solutions of the associated eigenvalue equation with energies in the continuum, which decay asymptotically, these solutions satisfy Eq. (A.2) but not Eqs. (2.9). They would be required for completeness but would not be included if the boundary conditions given by Eqs. (2.9) are adopted. A calculation of α_θ and β_θ would have to take into account the additional bound state solutions, thereby possibly complicating the problem considerably. We note, however, that if these additional solutions are orthogonal to the function we are expanding (i.e., the difference function w) their omission is of no consequence in an application of the Kato method.

Now bound-state solutions embedded in the continuum exist by virtue of their belonging to a different symmetry class from the scattering solutions and consequently being orthogonal to them. If the trial function is chosen with the correct symmetry properties then w will be orthogonal to the additional decaying solutions. Difficulties may arise if the true scattering solution has symmetry properties which are not easily recognizable. (Such difficulties are of course not peculiar to the Kato method; they exist for the ordinary variational principle as well.) We do not believe that any hidden symmetries exist in the e^+H problem. In any event, as we have already noted, we are able to claim complete rigor for the bound we have obtained on the e^+H scattering length, aside from any questions of completeness, by virtue of our having given an independent proof of the validity of the bound.

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Measurement of the Total, Differential, and Exchange Cross Sections for the Scattering of Low-Energy Electrons by Potassium*†

KENNETH RUBIN,‡ JULIUS PEREL, AND BENJAMIN BEDERSON
Department of Physics, New York University, University Heights, New York, New York

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An atom beam recoil technique has been used to determine the total, Q, differential, $\sigma(\theta)$, and differential exchange, $\sigma_e(\theta)$, cross sections for the scattering of low-energy electrons by potassium. The method consists of observing the angular distribution of atoms scattered from a potassium atom beam which has been cross fired by an electron beam. Relative values of $\sigma(\theta)$ are then obtained by transforming to electron scattering angles. An inhomogeneous magnet and collimating channel are used as a velocity filter for the atom beam. Curves representing the variation of $\sigma(\theta)$ with θ between approximately 15° and 60° are presented for various electron energies between 0.6 and 9.0 ev.

The magnet also serves to polarize the beam. Relative values of $\sigma_e(\theta)$ were determined by observing the amount of depolarization of the beam in the scattering region, using a second inhomogeneous magnet as an analyzer. Over the observed range of angles, exchange accounts for approximately one third of the scattering. Bounds on the total exchange cross section, Q_e, are also tabulated for energies between 0.5 and 4.0 ev. The bounds on Q_e at 0.5 volt are 0.8×10^{-14} cm$^2<Q_e<1.6\times10^{-14}$ cm^2.

1. INTRODUCTION

THE exchange interaction during an electron-atom scattering event plays a significant role in many scattering processes. Such interactions, however, have not been extensively studied. In some recent experiments performed by Dehmelt,[1] Novick and Peters,[2] and Franken *et al.*,[3] bounds on the cross sections for exchange scattering of thermal electrons by alkali atoms have been obtained. In these experiments, exchange cross sections were determined by observing depolarization by free electrons of an alkali gas previously aligned by optical pumping.

The main purpose of the present experiment was to observe exchange events directly by cross firing a polarized atom beam with a monoenergetic electron beam. Exchange collisions result in a readily observable partial depolarization of the atom beam. The method thus makes it possible to study exchange scattering as a function of electron energy. Furthermore, because of the recoil suffered by scattered atoms, these can readily be distinguished from the unscattered atom beam.[4,5] It is, therefore, possible to investigate differential scattering by observing the angular distribution of the scattered atoms.

By the use of this method, we have determined relative values of the differential cross section $\sigma(\theta)$ and the differential exchange cross section $\sigma_e(\theta)$ for the scattering of potassium by electrons over a range of

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