

Optical-Model Analysis of Low-Energy Electron-Hydrogen Scattering*

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The electron-hydrogen scattering problem is reduced to an equivalent one-body problem by the use of an optical-model potential. Two effects are examined quantitatively: the influence of the Pauli principle and the elastic scattering in the triplet state. For a long-range optical potential, the effect of the Pauli principle is small; however, for a short-range optical potential, the Pauli principle changes the zero-energy cross section by an order of magnitude.

The elastic scattering results, though in agreement with many previous calculations, are disappointing. It is argued that this is due to an inconsistent application of the optical model, and that a more consistent use of the optical model is equivalent to (and therefore provides a derivation for) the heuristic procedure, used by Martin, Seaton, and Wallace, which yields scattering lengths close to the Rosenberg, Spruch, and O'Malley bounds.

1. INTRODUCTION

THE success of optical-model techniques in nuclear physics—where their use is well known¹—suggests that these methods might also be of value in atomic scattering problems. This application of optical-model theory has already been considered, in its formal aspects, in two recent papers^{2,3}; in this paper, we describe its application to a practical, numerical problem—the elastic scattering of electrons by atomic hydrogen. A brief outline of our method is presented in this section, the detailed discussion being reserved for the later parts of this paper.

The optical model asserts an equivalence between a many-body problem and a one-body problem. The equivalence is achieved by replacing the many-body potential by an equivalent one-body potential—the “optical-model potential.” Unfortunately, this can be done exactly only when the solution to the many-body problem is known exactly; that is, a complete specification of the optical-model potential demands a complete solution of the scattering problem that the optical model simulates.

In our problem, although the complete expression of the optical-model potential, valid everywhere, is not known, its asymptotic form is available and is increasingly correct as we approach the limit where the adiabatic approximation^{4,5} holds, namely, large separation between the scattered electron and the atomic system. The proper expression for the optical potential is unknown only at small separation distances.

We have dealt with this circumstance, which seems to preclude the use of an optical potential, by constructing

the potential in two parts: the asymptotically correct, long-range part and the remaining, shorter-range part. The short-range part is represented by a function arbitrary in form, but of limited range. This part is introduced with a multiplicative factor that is adjusted by imposing, on the optical-model wave function, an orthogonality condition that the exact wave function is known to obey. The ensuing one-body scattering problem is then integrated numerically on a computing machine.

The orthogonality condition we employ arises naturally in the problem. For singlet scattering (total electronic spin function antisymmetric), it expresses the orthogonality of the scattering and the H^- wave functions. For triplet scattering (total electronic spin function symmetric), it is equivalent to the Pauli principle.

In the latter case, since we can impose the orthogonality requirement or ignore it at will, we obtain, in the normal course of our calculation, a quantitative estimate of the influence of the Pauli principle on low-energy electron-hydrogen scattering. These results, which have already been presented in preliminary form,⁶ are described more fully in Sec. 6a.

The wave function that emerges after the machine integration of the optical-model wave equation represents, to some unknown degree of approximation, a solution to the original scattering problem. Cross sections and other information can be obtained by using this wave function directly. However, we can also use this wave function as a trial function in a variational calculation. This procedure helps to compensate for some of the approximations that entered into the trial function. Thus, our philosophy is to regard the entire optical-model construction primarily as providing a rational basis for our choice of a trial function to be used in a variational principle; or, alternatively, the variational principle can be regarded as supplying the corrections that the wave function requires, due to the neglect of nonadiabatic and other effects.

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¹ See, for example, proceedings of the International Conference of the Nuclear Optical Model, Mar. 16–17, 1959 (Florida State University Studies No. 32), Florida State University, 1959.

² M. H. Mittleman and K. M. Watson, *Phys. Rev.* **113**, 198 (1959).

³ B. A. Lippmann, M. H. Mittleman, and K. M. Watson, *Phys. Rev.* **116**, 920 (1959).

⁴ B. H. Bransden, A. Dalgarno, J. L. John, and M. J. Seaton, *Proc. Phys. Soc. (London)* **71**, 877 (1958).

⁵ B. A. Lippmann, *Bull. Am. Phys. Soc.* **5**, 119 (1960).

⁶ B. A. Lippmann and H. M. Schey, *Bull. Am. Phys. Soc.* **5**, 378 (1960).

2. THE OPTICAL MODEL

The electrons in our problem are labeled 1 and 2, and the proton is considered to be infinitely heavy. The Schrödinger equation is

$$(E-H)\psi(1,2)=0, \quad (1)$$

where

$$\begin{aligned} H &= H_0 + V, \\ H_0 &= T_1 + T_2 - \frac{e^2}{|\mathbf{r}_1|}, \\ T_1 &= \mathbf{P}_1^2/2m; \quad T_2 = \mathbf{P}_2^2/2m, \\ V &= -\frac{e^2}{|\mathbf{r}_2|} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}. \end{aligned} \quad (2)$$

The symbols have their conventional meanings.

Equations (1) and (2) form a complete specification of the scattering problem, if we add the boundary condition

$$r_2 \rightarrow \infty: \psi(1,2) \sim \phi_1(1) \{ (e^{i\mathbf{k}_1 \cdot \mathbf{r}_2}) + \text{outgoing scattered waves in electron 2} \}. \quad (3)$$

The following additional remarks should be adjoined to Eq. (3). First, elastic scattering only has been assumed and spin functions have been suppressed. Second, the Pauli principle applied to (3), supplies the form of the boundary condition $r_1 \rightarrow \infty$. Finally $\phi_1(1)$ is the wave function of electron 1 in the ground state of hydrogen, and \mathbf{k}_1 is the wave vector of the incident wave.

The hydrogen-atom Hamiltonian, H_H , and its eigenfunctions, ϕ_n , are defined by

$$H_H \phi_n(1) = \left[T_1 + \frac{e^2}{|\mathbf{r}_1|} \right] \phi_n(1) = E_n \phi_n(1). \quad (4)$$

The complete set of hydrogenic eigenfunctions defines an expansion of $\psi(1,2)$, namely,

$$\begin{aligned} \psi(1,2) &= \sum_n \phi_n(1) \chi_n(2), \\ \chi_n(2) &= \langle \phi_n(1), \psi(1,2) \rangle_1. \end{aligned} \quad (5)$$

Here, the notation $\langle \cdots \rangle_1$ means that only electron 1 is involved in the Hermitian scalar product; if both electrons are involved, we shall use the usual notation in which the subscript is absent.

By definition, the optical-model wave function is χ_1 . According to (3), it is the only one of the χ_n 's that survives as r_2 approaches ∞ . Furthermore, taking the scalar product of (1) with $\phi_1(1)$, we see that, if we define the optical-model potential, $\mathcal{U}(2)$, by the relation

$$\mathcal{U}(2) \chi_1(2) \equiv \langle \phi_1(1), V \psi(1,2) \rangle_1, \quad (6)$$

then the optical-model wave function satisfies the Schrödinger equation

$$[(E - E_1) - T_2 - \mathcal{U}(2)] \chi_1(2) = 0, \quad (7)$$

where the boundary condition on $\chi_1(2)$ may be obtained by taking the scalar product of $\phi_1(1)$ and (3).

Equation (6) emphasizes the fact, mentioned in the Introduction, that the determination of the optical potential implies that the solution of the scattering problem is known.

Now, in the limit $r_2 \rightarrow \infty$, as we see from (2), V becomes very small. As this limit is approached, the solution of the scattering problem by first-order perturbation theory becomes more and more accurate. The exact wave function,

$$\psi(1,2) = \phi_1(1) \chi_1(2) + \sum_{n \neq 1} \frac{\phi_n(1) \langle \phi_n(1), V \psi(1,2) \rangle_1}{E - T_2 - E_n},$$

can be represented to first order by inserting $\phi_1(1) \chi_1(2)$ for $\psi(1,2)$ on the right. Using this expression for $\psi(1,2)$ in (6), we find

$$\begin{aligned} \mathcal{U}(2) &= \langle \phi_1(1), V \phi_1(1) \rangle_1 + \sum_{n \neq 1} \langle \phi_1(1), V \phi_n(1) \rangle_1 \\ &\quad \times \frac{1}{E - T_2 - E_n} \langle \phi_n(1), V \phi_1(1) \rangle_1 + \cdots \end{aligned} \quad (8)$$

The first term is the shielded Coulomb potential,

$$V_s(r) = -e^2 \left(\frac{1}{a_0} + \frac{1}{r} \right) e^{-2r/a_0}, \quad (9)$$

where $a_0 (= \hbar^2/mc^2)$ is the Bohr radius.

The second term of (8), evaluated in the adiabatic approximation ($E - T_2 \approx E_1$), which entails a negligible error for r_2 large,⁵ is

$$V_p(r) = -\alpha/2r^4. \quad (10)$$

Here α , the polarizability of the hydrogen atom, has the value⁷ 4.5. We emphasize that the expression (10) for the polarization potential is valid only in the limit where r_2 is very large.

Thus, in the limit of large r_2 the optical potential is known, namely,

$$r_2 \rightarrow \infty: \mathcal{U}(2) \sim V_s(r_2) + V_p(r_2), \quad (11)$$

and therefore the Schrödinger equation for χ_1 , Eq. (7), is also known in this region.

For r_2 small, the optical-model potential is unknown. Both the perturbation expansion and the adiabatic approximation break down in this region. If the adiabatic approximation breaks down first, $\mathcal{U}(2)$ becomes nonlocal, for then the T_2 in (8) can no longer be ignored.

In order to solve (7), we require $\mathcal{U}(2)$ for all values of r_2 . Our procedure will be to use (11) for r_2 large and to try to infer the optical potential for r_2 small by invoking properties the correct χ_1 is known to possess.

Thus, in place of (7) we shall use

$$[(E - E_1) - T_2 - \mathcal{U}(2)] \chi_1(2) = \lambda f(2), \quad (12)$$

⁷ A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. (London) **A233**, 70 (1955).

where $\mathcal{U}(2)$ is given by (11), and $f(2)$ is arbitrary in form, though it must be short-range so that (12) shall reduce, asymptotically, to (7). We have chosen the hydrogenic ground-state function, $\phi_1(2)$, for $f(2)$. The inhomogeneous term, $\lambda f(2)$, is similar to an exchange potential or other nonlocal potential, since it can be considered to be the result of an integral operator operating on χ_1 . The form given in (12) approximates the effect of an integral operator without making it necessary to solve an integrodifferential equation.

The λ in (12) is a parameter. It is adjusted to enable χ_1 to satisfy an orthogonality condition that the exact χ_1 is known to obey. This is explained in the next section.

3. THE ORTHOGONALITY CONDITION

(a) Triplet Scattering

Consider the scalar product of ϕ_1 and χ_1 . From (5), we have

$$\langle \phi_1(2), \chi_1(2) \rangle_2 = \langle \phi_1(2) \phi_1(1), \psi(1,2) \rangle = 0, \quad (13)$$

since the Pauli principle requires that the triplet $\psi(1,2)$ must be antisymmetric in the electronic coordinates. Thus, for triplet scattering the parameter λ in Eq. (12) may be adjusted to insure that χ_1 is orthogonal to the ground state of hydrogen. Further details are given in Sec. 5.

(b) Singlet Scattering

The condition (13) is no longer applicable in this case, for the singlet $\psi(1,2)$ is symmetric in the electronic coordinates. However, another orthogonality condition can be used to replace (13), namely, the requirement that the scattering wave function must be orthogonal to the H^- wave function, ψ_{H^-} , which is also a singlet wave function but belonging to a different energy. Or, if only the first term in the expansion (6) is used, λ is fixed by the requirement that

$$\langle \phi_1(1) \chi_1(2), \psi_{H^-}(1,2) \rangle = 0. \quad (14)$$

Note that because of the symmetric nature of ψ_{H^-} , only the symmetric part of $\phi_1(1) \chi_1(2)$ really is affected by (14).

4. THE VARIATIONAL PRINCIPLE

After solving Eq. (12), subject to (13) or (14) as the case requires, the asymptotic form of χ_1 is examined and from this the scattering cross section is inferred. The value thus obtained has been called the "direct calculation."

We have also constructed the function

$$\phi_1(1) \chi_1(2) - \phi_1(2) \chi_1(1), \quad (15)$$

and used it as a trial function in the Kohn variational principle.⁸ This is in keeping with our expectation,

⁸ W. Kohn, Phys. Rev. **74**, 1763 (1948).

already discussed, that errors arising from nonadiabatic and other effects could thereby be corrected in some measure. The variational principle was used to compute each partial wave separately, as discussed in Sec. 5, the cross sections obtained in this way being labeled "variational calculation."

The normalizations of the wave functions used in the variational calculations were adjusted as prescribed by Spruch and Rosenberg.⁹ This has the effect of making the triplet scattering lengths, computed variationally, upper bounds on the true scattering lengths.

5. COMPUTATIONAL DETAILS

To solve (12) we expand the wave function $\chi_1(\mathbf{r})$ in eigenstates of angular momentum. Putting

$$\chi_1(\mathbf{r}) = \sum_{l=0}^{\infty} u_l(r) P_l(\cos\theta),$$

we find that the radial functions $u_l(r)$ satisfy the equations

$$\frac{d^2 u_l}{dr^2} + \left[k_1^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} \mathcal{U}(r) \right] u_l(r) = \frac{2m\lambda}{\hbar^2} r f(r) \delta_{l0}, \quad (16)$$

where

$$k_1^2 = (2m/\hbar^2)(E - E_1).$$

Since we have considered only spherically symmetric functions $f(r)$, only the $l=0$ case of (16) contains an inhomogeneous term.

The boundary conditions on $\chi(r)$ may be translated into conditions on $u_l(r)$. Thus we require that $u_l(r)$ vanish at the origin and have only outgoing scattered waves at infinity. The orthogonality condition (13) may also be written in terms of the radial functions (of course, only the $l=0$ case will be involved):

$$\int_0^\infty u_0(r) r f(r) dr = 0. \quad (17)$$

To solve (16) we replace it by an equivalent difference equation according to standard procedures.¹⁰ The difference equation is then solved numerically on an IBM-704 computer subject to the boundary conditions. The procedure involves integrating numerically from $r=0$ to $r=r_{\max}$ at and beyond which the optical potential and the inhomogeneous term $r f(r)$ are essentially zero. At this point the numerical solution is joined smoothly to a linear combination of spherical Bessel functions which is the solution in the field-free region. The scattering-phase shifts, from which the cross section is calculated, are, of course, determined from the asymptotic form of the wave function.

⁹ L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959); **117**, 1095 (1960).

¹⁰ See, for example, B. J. Scarborough, *Numerical Mathematical Analysis* (Johns Hopkins Press, Baltimore, Maryland, 1955), 3rd ed., pp. 265 ff.

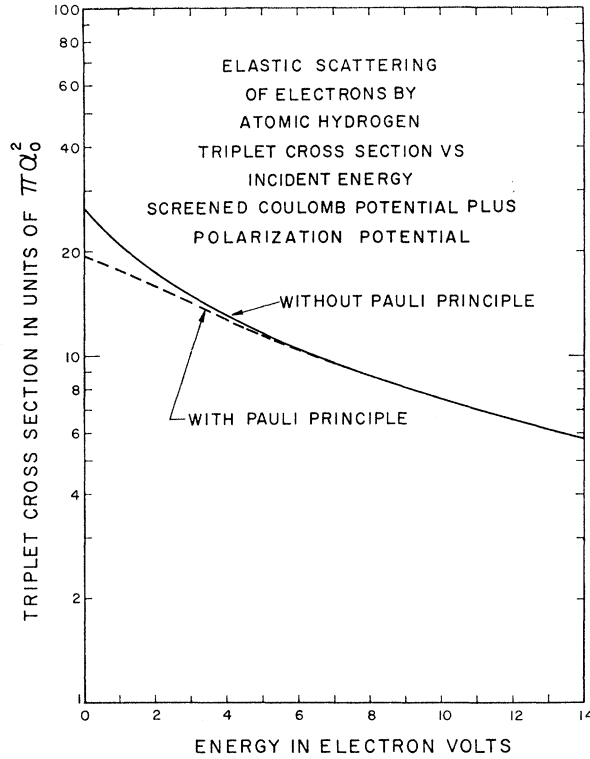


FIG. 1. Effect of Pauli principle on scattering by a long-range potential.

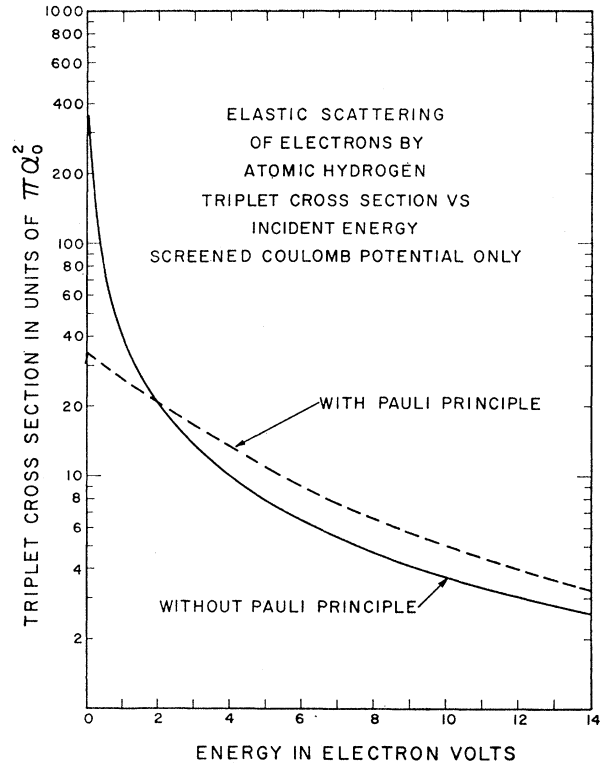


FIG. 2. Effect of Pauli principle on scattering by a short-range potential.

In order to fulfill the orthogonality requirement [Eq. (17)] we follow the above procedure twice in the case $l=0$. The equation is first integrated with $\lambda=0$, yielding the solution $u_0^{(0)}(r)$, and then a second time with $\lambda=1$ to give $u_0^{(1)}(r)$. The general solution for arbitrary λ is then clearly

$$u_0(r) = cu_0^{(0)}(r) + \lambda u_0^{(1)}(r), \quad (18)$$

where c is some constant. Equation (17) may now be rewritten

$$c \int_0^\infty u_0^{(0)}(r) r f(r) dr + \lambda \int_0^\infty u_0^{(1)}(r) r f(r) dr = 0.$$

With c given in terms of λ according to this relationship, the $l=0$ solution, Eq. (18), satisfies the orthogonality requirement. The solution, of course, is normalized arbitrarily, but this is irrelevant for the determination of the phase shift.

Once (16) has been solved we are in a position to make a calculation based on a variational principle. We write the Kohn variational principle for each angular momentum state in the form

$$\tan \delta_l = \tan \delta_l' + \frac{(2l+1)m}{4\pi\hbar^2 k_1} I_l,$$

where δ_l' is the l th partial wave phase shift resulting

from the direct calculation described above, and

$$I_l = \int \psi_l(E-H)\psi_l d\mathbf{r}_1 d\mathbf{r}_2, \quad (19)$$

where

$$\psi_l = \phi_1(r_1) \frac{u_l(r_2)}{r_2} P_l(\cos \theta_2) - \phi_1(r_2) \frac{u_l(r_1)}{r_1} P_l(\cos \theta_1)$$

is the l th partial wave term of (15). The functions $u_l(r)$ are normalized according to Rosenberg and Spruch's prescription, and δ_l is, of course, the "corrected" phase shift predicted by the variational principle. The angular integrations involved in (19) are easily carried out analytically, and the remaining integrations over the radial variable are performed numerically using Simpson's rule.

6. RESULTS

As we have seen, for triplet scattering the Pauli principle reduces to the orthogonality condition (13). Equation (12) was integrated for two optical potentials, $\mathcal{V} = V_s + V_p$ and $\mathcal{V} = V_s$. In each case, a solution was found with the Pauli principle included [λ chosen to satisfy (13)], and with the Pauli principle ignored [$\lambda=0$ in (12)]. V_p was taken to be $-\alpha/2(r^2+d^2)^2$, with $d=1.5a_0$. This has the correct asymptotic form and is finite at the origin. The values of the cross section that resulted are plotted in Figs. 1 and 2.

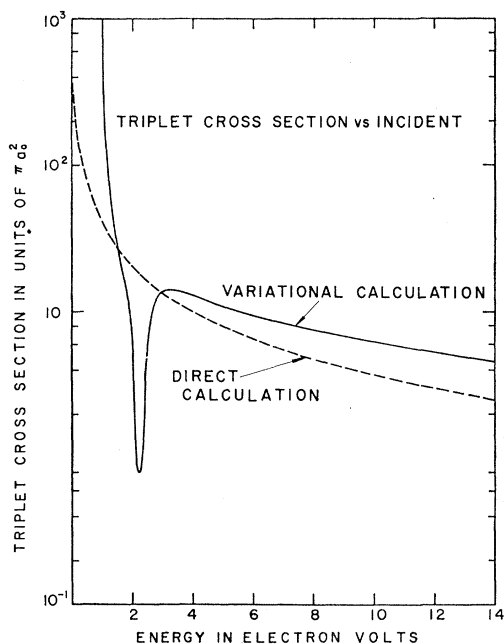


FIG. 3. Electron-hydrogen scattering, according to the optical model, using only the screened Coulomb potential as the optical potential. Pauli principle ignored.

According to general principles, one expects that the effect of the Pauli principle would be small at large energies and large at small energies. Figure 1 tends to confirm this expectation: The effect of the Pauli principle is greatest at zero energy, and it becomes unobservably small as the energy increases. Figure 2,

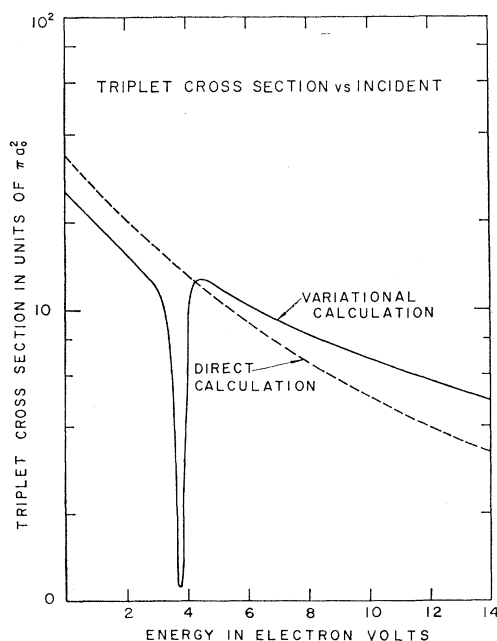


FIG. 4. Electron-hydrogen scattering, according to the optical model, using the screened Coulomb potential as the optical potential and including the Pauli principle.

however, seems anomalous; although the Pauli principle changes the zero-energy cross section much more than the cross sections at any other energy, the effect does not diminish with increasing energy, as in Fig. 1.

The explanation of this behavior is obtained by noting that the overlap of the wave functions of the two electrons determines the influence of the Pauli principle. If the overlap is large, the effect of the Pauli principle is large; if the overlap is small, so is the effect of the Pauli principle. Now, as the energy increases, the electrons can be represented by more and more highly localized wave packets. The overlap then is negligible except when the electrons are very close to one another. In Fig. 1, a long-range potential, V_p , is present. Most of the scattering occurs before the electrons are very close, i.e.,

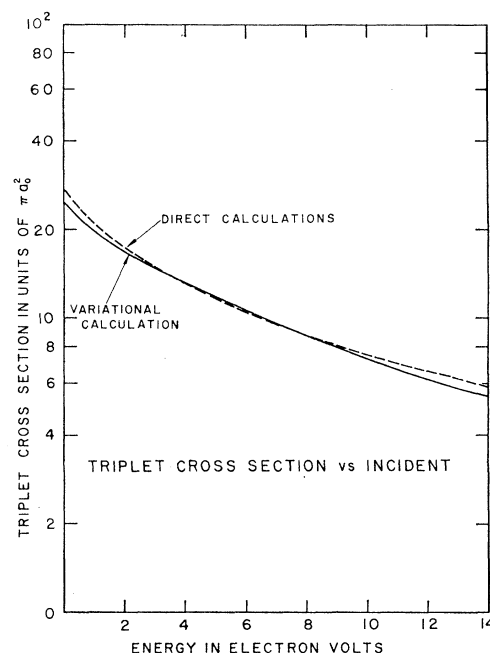


FIG. 5. Electron-hydrogen scattering, according to the optical model, using the screened Coulomb potential and the polarization potential as the optical potential. Pauli principle ignored.

most of the scattering takes place far from the overlap region. For this reason, the Pauli principle is negligible at high energies, when the overlap region can be made very small, and has only a moderate effect at low energies, when the overlap region becomes comparable to the range of the potential.

In Fig. 2, on the other hand, the potential is quite short in range. The Pauli principle has a large effect—an order of magnitude at zero energy—because now almost all the scattering occurs when the electrons are close together. Even at the energies considered, the overlap of the wave packets is about the same as the range of the potential; thus the Pauli principle has a noticeable effect over the entire range of energies shown, although its influence is particularly large at zero energy.

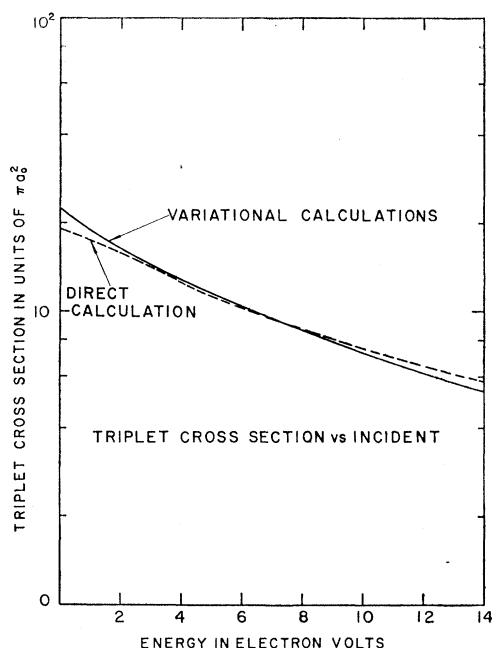


FIG. 6. Electron-hydrogen scattering, according to the optical model, using the screened Coulomb potential and the polarization potential as the optical potential and including the Pauli principle.

The curves of Figs. 1 and 2, which correspond to a "direct calculation," are replotted in Figs. 3-6, each together with the associated "variational calculation."

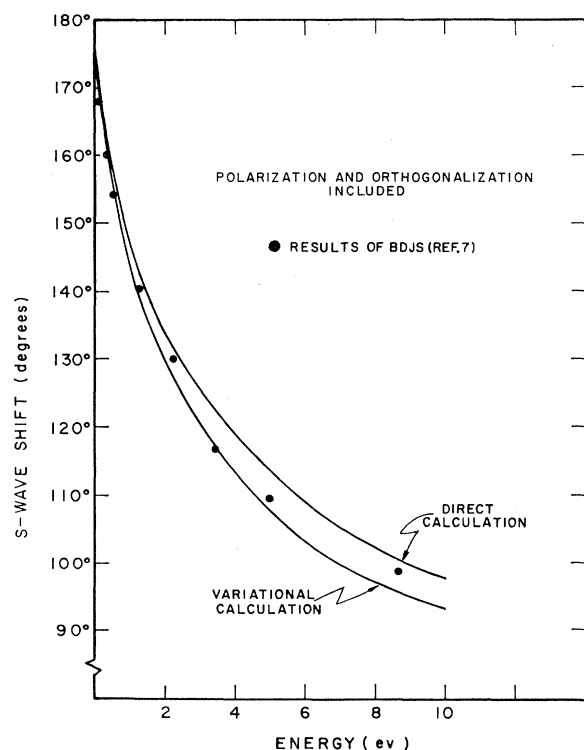


FIG. 7. *S*-wave phase shift corresponding to the variational calculation of Fig. 6.

We have several comments concerning these last four figures.

1. Figures 3 and 4 show rather striking dips in the variational results, around 2-4 volts. These sharp minima are a consequence of the *S*-wave phase shifts passing through zero. Without going into details, we remark that we regard these dips as spurious. The other portions of these curves are dependable.

2. The variational results of Figs. 4-6 lie very close to one another. This is particularly true of Figs. 5 and 6; if superimposed, these curves coincide exactly except in the region 0-2 volts, where they differ slightly.

According to the Rosenberg-Spruch theorem,⁹ zero energy is a critical point for the variational calculations: The variational calculation that produces the smallest scattering length at zero energy is the most accurate. This criterion, applied to the set of scattering lengths tabulated in Table I, suggests that the calculation plotted in Fig. 6 is the most accurate of the variational calculations.

3. The direct calculations of Figs. 5 and 6 give different results at zero energy. The corresponding variational results also differ, but by a much smaller amount;

TABLE I. Triplet scattering lengths.

	Direct calculation	Variational calculation
Pauli principle ignored	$2.60a_0$	$2.48a_0$
Pauli principle included	$2.19a_0$	$2.39a_0$

that is, the variational principle displaces the diverging direct calculations towards each other. The magnitudes of the displacements suggest that we are converging on a wave function that makes the variational expression stationary, but we have no assurance that this is the exact solution; what is more likely is that we are converging on the best solution—in a variational sense—that is possible for a trial function of the assumed form.

4. The *S*-wave phase shifts plotted in Fig. 7 have been taken from our most dependable variational calculation, that belonging to Fig. 6. The phase shift given by the associated direct calculation is also shown, together with a set of phase shifts adopted, after a critical analysis of several calculations, by Bransden, Dalgarno, John, and Seaton.¹¹ We note that their points agree very well with our variational calculation, but, again, we cannot infer from this that we are converging on the exact solution.

Indeed, we know, from recent work by Rosenberg, Spruch, and O'Malley,¹² that the zero-energy triplet scattering length is no more than $1.91a_0$. Our value of

¹¹ Reference 4, Table VI.

¹² L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **119**, 164 (1960).

$2.39a_0$ shows that our trial function has an error of at least 50%.

A triplet scattering length of 1.99 has been calculated by Martin, Seaton, and Wallace,¹³ using an equation which, they say, "cannot be derived from a consistent variational argument." Their method of calculation differs from ours in only two respects: First, they use an exchange potential in Eq. (12) instead of the $\lambda\phi_1$ term that we use; and second, in Eq. (15) they replace ϕ_1 by

$$\phi_1(2) + \sum_{n \neq 1} \phi_n(2) \frac{\langle \phi_n(1), V\phi_1(1) \rangle_1}{E_1 - E_n}, \quad (20)$$

where, in the actual numerical evaluation, they include $2p$ states only in the sum over n . The extra term in (20) is, of course, the first-order perturbation-theoretic correction to ϕ_1 evaluated in the adiabatic approximation.

The use of an exchange potential instead of $\lambda\phi_1$ should not cause the Martin, Seaton, and Wallace results to deviate significantly from ours, since both the exchange potential and the $\lambda\phi_1$ term serve only to satisfy the Pauli principle. We therefore infer from the Martin, Seaton, and Wallace calculation, that the use of (20) in our calculation would improve our estimate of the triplet scattering length, bringing it close to the present upper bound established by Rosenberg, Spruch, and O'Malley. Furthermore, it is clear (after the fact) that the replacement of ϕ_1 by (20) is really necessary in our calculation: having already used (20) to calculate the asymptotic form of the optical potential, consistency demands that (20) also be used in (15) in order that the asymptotic forms of the optical potential and the wave function both be considered to the same order of accuracy. In this sense, our method provides a rationale for the equation, established heuristically by Martin, Seaton,

¹³ V. M. Martin, M. J. Seaton, and J. B. G. Wallace, *Proc. Phys. Soc. (London)* **72**, 701 (1958). We are indebted to Professor Spruch for calling this calculation to our attention.

and Wallace. It is satisfying to see that such a simple procedure leads to scattering lengths close to the present limits established by the Rosenberg-Spruch theorem.^{14,15}

7. CONCLUSIONS

1. The Pauli principle is important only when the wave functions of the two electrons overlap. If the optical potential is long-range, and such that most of the scattering occurs far from the region of overlap, the Pauli principle has a small effect; if the potential is short-range, and such that scattering is appreciable only in the overlap region, the Pauli principle can change the zero-energy cross section by an order of magnitude.

2. The optical-model analysis of low-energy electron-hydrogen scattering, in its simplest form, leads to results in good agreement with previous calculations, but not at all close to the limits presently associated with the Rosenberg-Spruch theorem. However, it is suggested that a more consistent use of the optical model leads to a calculational procedure, very much like that already used by Martin, Seaton, and Wallace,¹³ which produces scattering lengths close to the upper bounds established by Rosenberg, Spruch, and O'Malley.¹²

ACKNOWLEDGMENTS

It is a pleasure to acknowledge our indebtedness to Professor K. M. Watson, who suggested the Pauli principle calculation, and to Douglas Jeung, who coded, for the IBM-704, all the computations reported in this paper.

¹⁴ Although we have discussed only the triplet scattering explicitly, these remarks also apply to the singlet scattering. In this case, too, the Bransden, Dalgarno, John, and Seaton calculation gives a result close to the upper bound found by Rosenberg, Spruch, and O'Malley.

¹⁵ We note that the use of (20) is also the starting point for procedures employed by A. Temkin and J. Lamkin, *Phys. Rev.* **121**, 788 (1961), where, again, it leads to scattering lengths close to the Rosenberg, Spruch, and O'Malley values.