

## Low-Energy Scattering of a Charged Particle by a Neutral Polarizable System\*

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In the scattering of a particle (or system) of charge  $Ze$  by a neutral system with an electrical polarizability  $\alpha$ , an electric dipole moment is induced which generates an effective potential that behaves asymptotically as  $-\frac{1}{2}Z^2e^2\alpha/r^4$ . Due to this effective long-range interaction, effective-range theory in its normal form is not applicable. Thus, for the scattering of a particle with an incident orbital angular momentum of zero, for example, the expansion of  $k \cot\eta(0)$  includes terms in  $k$  and in  $k^2 \ln k$ , in addition to the usual constant and  $k^2$  terms. The effective range  $r_0$  as normally defined is infinite, but one can define a quantity  $r_{p0}$  which explicitly takes into account the long-range character of the effective potential. For  $L > 0$  it is  $k^2 \cot\eta(L)$  which approaches a constant as  $k$  approaches zero rather than  $k^{2L+1} \cot\eta(L)$  as for a short-range potential. The above results can have serious consequences in the scattering of electrons and of positrons by neutral spherically symmetric atoms. Some detailed consideration is given to the scattering by hydrogen atoms. The formulation of effective-range theory which is given is valid when Pauli exchange between the two colliding systems is possible. The method used for taking into account the effect of the Pauli principle (this method would be the same for long-range and short-range forces) is rather more convenient than in the usual presentation of effective range theory.

### 1. INTRODUCTION

EFFECTIVE-range theory (ERT), which gives the leading terms in the expansion of  $k^{2L+1} \cot\eta(L)$  as a power series in  $k^2$ , where  $\eta(L)$  is the phase shift for angular momentum  $L$ , was originally developed<sup>1</sup> for the analysis of nucleon-nucleon scattering. For  $n$ - $n$  or  $n$ - $p$  scattering, the potential is the short-range nuclear potential; for  $p$ - $p$  scattering, the potential is the short-range nuclear potential plus the long-range Coulomb potential, but the effects of the Coulomb field can be accounted for explicitly, and once again the phase shift that enters into effective-range theory is that due to a short-range potential, though the phase shift is measured relative to pure Coulomb scattering.

For the scattering of neutral particles by a compound system which contains particles identical with the incident particle (neutrons on nuclei affords an example),<sup>2</sup> the only new feature is that the Pauli principle enters in a rather more complicated and significant way than it does for  $n$ - $n$  or for  $p$ - $p$  scattering. This more complicated case has been treated in the literature, but the treatment has either been not quite correct or else<sup>3</sup> it has been rather less simple than is possible, in that a redundant element is introduced. This situation is analyzed in Sec. 2.

A second and much more interesting feature enters

in the development of an ERT, or rather of a modified ERT, for the scattering of a charged particle (or system) by a neutral polarizable<sup>4</sup> system. [The Pauli principle may not (positrons on atoms, for example) or may (electrons on atoms, for example) be relevant here.] This feature is that at low energies, the domain of interest for ERT, the target system develops a dipole moment in the presence of the charged particle, so that the interaction between the charged particle and the target system has an asymptotic  $1/r^4$  dependence. In the presence of this long-range polarization potential the usual ERT breaks down and one must develop a modified ERT. It has been shown previously<sup>5,6</sup> that ERT breaks down for scattering by an asymptotic static central potential which vanishes as  $1/r^4$ . No such static central potentials are of much significance and the case was studied primarily because an effective interaction whose dominant long-range term goes as  $1/r^4$  arises in the scattering of a charged particle by a neutral spherically symmetric atom. It is shown in Sec. 3 that the modification of ERT previously introduced for the central potential case is in fact valid for the scattering of electrons or positrons by atoms, in the following sense. In scattering by an atom, the  $1/r^4$  term is only the leading term in the effective long-range interaction. There are other long-range interactions as well. To make contact with the results for the static potential case as treated in reference 6, it will sometimes be necessary to arbitrarily neglect the other long-range interactions.

It should not be thought that the difficulty in making

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<sup>1</sup> J. M. Blatt and J. D. Jackson, *Phys. Rev.* **76**, 18 (1949); J. D. Jackson and J. M. Blatt, *Revs. Modern Phys.* **22**, 77 (1950); H. A. Bethe, *Phys. Rev.* **76**, 38 (1949); G. F. Chew and M. L. Goldberger, *Phys. Rev.* **75**, 1637 (1949).

<sup>2</sup> We ignore here the electrical polarizability of the neutron; see R. M. Thaler, *Phys. Rev.* **114**, 827 (1959).

<sup>3</sup> T. Ohmura, Y. Hara, and T. Yamanouchi, *Progr. Theoret. Phys. (Kyoto)* **20**, 80 (1958).

<sup>4</sup> The word "polarizability" is used in the literature in many ways. In neutron-deuteron scattering, for example, one might speak of the polarizability of the deuteron, polarizability and distortion being interchangeable in this usage. In the present paper, we reserve the word "polarizability" for electrical polarizability.

<sup>5</sup> L. Spruch, T. F. O'Malley, and L. Rosenberg, *Phys. Rev. Letters* **5**, 347 (1960).

<sup>6</sup> T. F. O'Malley, L. Spruch, and L. Rosenberg, *J. Math. Phys.* **2**, 491 (1961). The notation Eq. (I-...) will refer to equations in this paper.

contact arises because of the many-body character of the scattering. Rather the point is simply that the central potential considered<sup>6</sup> was assumed to vanish as  $1/r^4$ , with no other long-range components. To the extent that a modified ERT can be obtained for the central potential problem in which the long-range interaction is a specified sum of powers of  $1/r$ , the form of the modified ERT will be known for scattering by a compound system for which the effective long-range interaction is that same specified sum. Of course, the determination of the actual numerical values of the various coefficients will be much more complicated for scattering by a compound system.

The restriction to just a  $1/r^4$  term arose naturally in our previous paper<sup>6</sup> from the mathematical approach. The recognition that the mathematical solutions of the Schrödinger equation in which the potential is equal to a multipole of  $1/r^4$  for all  $r$  is a known function, the Mathieu function, reduces the problem of the development of a modified ERT to the problem of finding the various necessary expansions of the Mathieu function in a treatise on that function. Were these expansions not known, one would have to develop them. For a potential with a number of long-range interactions, the modified ERT can be readily obtained if one can determine the similar but algebraically more complicated expansion. There is every reason to believe that this determination is possible, as evidenced by some preliminary work in the development of the appropriate asymptotic expansions by J. B. Keller and B. Levy. We will not, however, use this more general approach in the present paper.

In the scattering of a charged particle (or system) by a *charged* polarizable system, the leading terms in the long-range interaction will be the Coulomb  $1/r$  term and the polarization  $1/r^4$  term. Once again ERT in its normal form, even as modified to include Coulomb effects, will break down. In line with our previous discussion, it should be possible to determine the appropriate modified ERT, but we have not as yet attempted to do so.

A very important example of long-range interactions arises in the scattering of a neutral polarizable system by a neutral polarizable system. For  $r$  large but not too large, the dominant term is the  $1/r^6$  Van der Waals' interaction, as a consequence of which ERT will have to be modified for larger values of  $L$ . In spite of its considerable interest, we will not consider this case.

We will always assume that the target system does not have a permanent dipole moment. Relativistic and magnetic effects will also be ignored, and the nucleus will be taken to have an infinite mass relative to that of an electron.

## 2. SHORT-RANGE POTENTIALS

### A. Incident Particle Distinguishable

We begin by considering the simplest possible example of the scattering of a particle by a compound system,

that for which the incident particle is distinguishable from the particles in the target (which may or may not be distinguishable from one another) and for which  $V'$ , the sum of the interactions between the incident particle and the target particles, is of short range. Here and elsewhere it will be assumed that the incident energy and the properties of the target and of the incident particle are such that (single-channel) elastic scattering is the only possible process. (As usual, to the extent of the validity of the approximation in which the electromagnetic interaction is turned off, we can include the case for which there are bound states of the composite system of the target plus the incident particle.)

The ground-state wave function  $F$ , the ground-state energy  $E_0$ , and the Hamiltonian  $H_0$  of the target system satisfy

$$(H_0 - E_0)F = 0. \quad (2.1)$$

$F$  depends upon the space and spin coordinates of the target particles. It has a specified value of the total angular momentum  $I$  and of the total angular momentum projection  $I_z$  of the target, and it vanishes as any target interparticle distance goes to infinity. The scattering wave function  $\Psi$  satisfies

$$(H_0 + T_q + V' - E)\Psi = 0, \quad (2.2)$$

where the center-of-mass motion has been separated out, where  $q$  is the distance between the incident particle and the center of mass of the target, where

$$T_q = -(\hbar^2/2\mu)\nabla_q^2,$$

and where

$$E = E_0 + \hbar^2 k^2 / (2\mu).$$

For zero incident energy, we have

$$(H_0 + T_q + V' - E_0)\Psi_0 = 0. \quad (2.3)$$

To simplify the discussion we restrict ourselves, in Sec. 2, to the case where the relative orbital angular momentum in the asymptotic region is zero,<sup>7</sup> and where the total angular momentum  $J$  and its  $z$  projection  $J_z$  satisfy  $J = J_z = I + S$ , with  $I$  and  $S$  representing the spins of the target system and the incident particle, respectively. The asymptotic forms of  $\Psi$  and of  $\Psi_0$  are then given by

$$\Psi \rightarrow F X_{ss} \sin[kq + \eta(0)] / [q \sin\eta(0)] \equiv \Psi^\infty, \quad \text{for } q \rightarrow \infty, \quad (2.4)$$

$$\Psi_0 \rightarrow F X_{ss} (1/q - 1/A) \equiv \Psi_0^\infty, \quad \text{for } q \rightarrow \infty, \quad (2.5)$$

where  $X_{ss}$  is the spin function of the incident particle and where it is here to be understood that  $F$  has  $I_z = I$ . The scattering length  $A$  is defined by Eq. (2.5). It will shortly be seen that it of course satisfies the usual

<sup>7</sup> As we have previously observed (reference 6), ERT with short-range potentials is simplest for the case of zero orbital angular momentum, though the distinction disappears when  $1/r^4$  potentials are introduced. Both of the above restrictions, to  $L=0$  and to short-range potentials, will be dropped in Sec. 3.

relationship

$$\lim_{k \rightarrow 0} k \cot \eta(0) = -1/A. \quad (2.6)$$

$\Psi$  and  $\Psi_0$  are both to vanish as any target interparticle coordinate goes to infinity. The significant feature for present purposes is that  $\Psi^\infty$  and  $\Psi_0^\infty$  are solutions of the homogeneous differential equations

$$(H_0 + T_q - E)\Psi = 0, \quad (2.7)$$

$$(H_0 + T_q - E_g)\Psi_0^\infty = 0. \quad (2.8)$$

Manipulating Eqs. (2.2), (2.3), (2.7), and (2.8) in a fashion almost identical with that used in the scattering by a center of force then leads to the identity of the standard form,

$$k \cot \eta(0) = -1/A + k^2 \int (\Psi^\infty \Psi_0^\infty - \Psi \Psi_0) d\tau, \quad (2.9)$$

where the integration is now over the coordinates of all of the particles. By the standard argument, we arrive finally at the ERT approximation

$$k \cot \eta(0) = -1/A + \frac{1}{2} r_0 k^2 + O(k^4), \quad (2.10)$$

where

$$\frac{1}{2} r_0 = \int [(\Psi_0^\infty)^2 - (\Psi_0)^2] d\tau. \quad (2.11)$$

The extension to this case therefore requires only the most trivial modifications.

When the incident particle and the target can form a composite bound state, the derivation of the expansion of  $k \cot \eta(0)$  about the energy of the bound state is once again almost identical in form with that for scattering by a central potential.

## B. Identical Particles

We now consider the extension to the case for which the incident particle is identical with some of the particles in the target; the interaction between the incident particle and the target particles will again be taken to be of short range. A prototype problem is the scattering of a neutron by a nucleus of  $A$  nucleons,  $Z$  protons, and  $N$  neutrons. The formalism will be developed for this problem.<sup>8</sup> The protons will be numbered 1 through  $Z$  and the neutrons  $Z+1$  through  $A+1$ . We define  $q_i$  as the distance of neutron  $i$  from the center of mass of the other  $Z+N$  particles,  $r_{mn}$  as the distance between particles  $m$  and  $n$ ,  $X_{ss}(i)$  as the spin function of the  $i$ th neutron,  $T$  as the sum of the kinetic energy operators with the center-of-mass motion separated out, and  $V$  as the sum of the potential energy interactions. The scattering functions  $\Psi$  and  $\Psi_0$ , which satisfy the equations

$$(T + V - E)\Psi = 0, \quad (2.12)$$

$$(T + V - E_g)\Psi_0 = 0, \quad (2.13)$$

<sup>8</sup> The notation will be patterned after that used by L. Spruch and L. Rosenberg, Phys. Rev. 117, 1095 (1960).

now take on the asymptotic forms

$$\begin{aligned} \Psi \rightarrow P_i(N+1)^{-\frac{1}{2}} F(-i) X_{\frac{1}{2}}(i) \\ \times \sin[kq_i + \eta(0)] / [q_i \sin \eta(0)] \equiv \psi_i^\infty \\ \text{for } q_i \rightarrow \infty, r_{mn} < \infty, m, n \neq i, \end{aligned} \quad (2.14)$$

$$\begin{aligned} \Psi_0 \rightarrow P_i(N+1)^{-\frac{1}{2}} F(-i) X_{\frac{1}{2}}(1/q_i - 1/A) \equiv \psi_{i0}^\infty, \\ \text{for } q_i \rightarrow \infty, r_{mn} < \infty, m, n \neq i. \end{aligned} \quad (2.15)$$

Here  $F(-i)$  is the ground-state wave function of the nucleus consisting of all  $A+1$  particles except neutron  $i$ . It is taken to be normalized to unity and antisymmetric in the proton and neutron coordinates separately; it is thus defined up to a factor  $-1$ . The  $P_i$  are constants which take the values  $\pm 1$  and may be so chosen, for a given definition of the sign of the  $F(-i)$ , (see, e.g., ref. 8) such that Eqs. (2.14) and (2.15) are asymptotic forms appropriate for functions which are antisymmetric in the  $Z$  proton and in the  $N+1$  neutron coordinates.

At this stage, it might seem natural to introduce

$$\sum_i \psi_i^\infty,$$

as the quantity which is to play the role of the asymptotic form of  $\Psi$ . It should be noted, however, that contrary to the situation in subsection A, this quantity does *not* satisfy any homogeneous differential equation. The origin of this difficulty lies in the fact that the different  $\psi_i^\infty$  satisfy homogeneous differential equations with different potentials dropped from the original full Hamiltonian. Each  $\psi_i^\infty$  does separately satisfy a homogeneous equation, namely,

$$[T + V(-i) - E]\psi_i^\infty = 0, \quad (2.16)$$

where  $V(-i)$  includes all interactions other than those which involve the  $i$ th neutron. We also have

$$[T + V(-i) - E_g]\psi_{i0}^\infty = 0. \quad (2.17)$$

We now manipulate Eqs. (2.12) and (2.13) in the usual fashion and we then do the same with each of the  $N+1$  pairs of equations, corresponding to the various possible values of  $i$ , Eqs. (2.16) and (2.17). Subtracting the sum over  $i$  of the latter results from the former, we arrive<sup>9</sup> at the sought-for identity

$$k \cot \eta(0) = -1/A + k^2 \int [\sum_i \psi_i^\infty \psi_{i0}^\infty - \Psi \Psi_0] d\tau. \quad (2.18)$$

We have finally the effective-range theory approximation:

$$k \cot \eta(0) = -1/A + \frac{1}{2} r_0 k^2 + O(k^4), \quad (2.19)$$

where

$$\frac{1}{2} r_0 \equiv \int [\sum_i (\psi_{i0}^\infty)^2 - (\Psi_0)^2] d\tau. \quad (2.20)$$

<sup>9</sup> The surface terms are handled in the standard way. See, for example, the rather similar situation treated in the derivation of Eq. (2.4) of reference 8.

Note that even though  $\Psi$  and  $\Psi_0$  each have  $N+1$  asymptotic components,  $\Psi\Psi_0$  also has only  $N+1$  asymptotic components, since components associated with different values of  $i$  are asymptotically nonoverlapping. It is for this reason that an asymptotic form for  $\Psi\Psi_0$  could be used in Eq. (2.18) which involved a single rather than a double sum. A similar remark holds for Eq. (2.20).

A case for which the incident particle is identical with the target particles and to which ERT has been applied<sup>3</sup> is the scattering of electrons by atomic hydrogen. Due to the existence of the long-range polarization potential, the applicability of ERT in its normal form to this example must be reexamined (see Sec. 3), but we are concerned in this section only with the effects of the Pauli principle. Their procedure was to construct an inhomogeneous differential equation satisfied by  $\sum_i \psi_{i0}^\infty$ , and their final form is

$$\frac{1}{2}r_0 = \int [(\sum_i \psi_{i0}^\infty)^2 - (\Psi_0)^2] d\tau + \text{Expl.} \quad (2.21)$$

where Expl. represents some terms that are given explicitly. They thus have a double sum rather than a single sum, plus additional terms. Examination of their results shows, however, that the cross terms in the double sum cancel the additional terms,<sup>10</sup> so that their result when simplified reduces to the form given by Eq. (2.20). In their analysis the various terms are rather simple and the additional difficulty introduced by the use of Eq. (2.21) rather than its simpler equivalent, Eq. (2.20), is negligible. On the other hand Mathieu functions are introduced when long-range effects are taken into account, and it is there important to recognize the cancellation and to use the appropriate long-range potential generalization of Eq. (2.20).

### 3. LONG-RANGE ( $1/r^4$ ) POLARIZATION INTERACTION

#### A. Incident Particle Distinguishable

We now consider the scattering of a charged particle by a neutral polarizable system whose particles may or may not be distinguishable from one another but are distinguishable from the incident particle. For reasons that will become apparent, we restrict our attention to neutral systems which are spherically symmetric. A prototype problem would be the scattering of positrons by a neutral spherically symmetric atom with atomic number  $Z$ . (The possibility of positron-electron annihilation will be ignored. In line with an earlier comment, the energy is of course to be sufficiently low so that neither pickup nor any other process but elastic scattering is possible.) For concreteness, we will consider this prototype problem.

The effective  $1/r^4$  interaction experienced by a charged particle in the presence of a polarizable system

<sup>10</sup>  $\psi_{i0}^\infty$  and  $\psi_{j0}^\infty$  for  $i \neq j$  are of course not orthogonal since they are solutions of equations involving different Hamiltonians.

is well known both classically and quantum mechanically, and its derivation has been given previously in a number of different contexts,<sup>11</sup> both in the adiabatic approximation and independently of this approximation. In order to establish a notation and to be able to stress those aspects relevant to the present problem, we will briefly summarize the derivation.

Let  $\mathbf{r}$  represent the position of the positron relative to the center of the atom. For the moment, in the spirit of the adiabatic approximation, we take  $\mathbf{r}$  to be fixed and study the effects on the ground-state wave function and on the energy of the atom of the presence of the positron.

The perturbation felt by the atom is then given by

$$H'(1, \dots, Z; \mathbf{r}) = -\sum_{i=1}^Z e^2/|\mathbf{r}-\mathbf{r}_i| + Ze^2/r. \quad (3.1)$$

Since we are only interested in large values of  $r$ , and since the probability of finding an electron at large  $r_i$  vanishes exponentially with  $r_i$ , we can neglect the possibility that  $r_i$  is larger than  $r$ , which gives

$$H' \approx -\sum_{l=1}^{\infty} (e^2/r^{l+1}) \sum_{i=1}^Z r_i^l P_l(\cos\theta_i), \quad (3.2)$$

where  $\theta_i$  is the angle between  $\mathbf{r}_i$  and  $\mathbf{r}$ . If the ground state of the atom has an electric quadrupole moment, the first-order perturbation energy will include a term, due to the  $l=2$  component of Eq. (3.2), which goes asymptotically as  $1/r^3$  and which will dominate over the  $1/r^4$  polarization potential which is the primary concern of the present paper. Unless otherwise noted, we will therefore restrict ourselves to atoms which do not have quadrupole moments, that is, to atoms which have a total angular momentum of zero or one-half.<sup>12</sup> We might note that an application of the formulas of this paper to electron scattering by the rare-gas atoms is now in progress.

For such atoms, and in the approximation given by Eq. (3.2), the first-order perturbation term for the energy is identically equal to zero. (The true  $H'$  gives a nonzero first-order term, but it is of short range.  $\mathbf{r}$  is held constant in these perturbation calculations.) Proceeding to the second-order energy term, we will for the moment rather arbitrarily retain only the leading  $l=1$  term. (The higher values of  $l$  generate terms the most significant of which is due to the  $l=2$  part of  $H'$  and vanishes asymptotically as  $1/r^6$ . We will discuss

<sup>11</sup> The treatment here is patterned after that of Sternheimer in his analysis of atomic polarizabilities. See R. M. Sternheimer, Phys. Rev. **96**, 951 (1954), and references to his earlier works contained therein.

<sup>12</sup> To the extent that orbital and spin angular momenta are also good quantum numbers, atoms with an orbital angular momentum of zero are of course also allowed, independent of the value of the spin.

these terms later.) We then have

$$H' \approx - (e^2/r^2) \sum_{i=1}^Z z_i, \quad (3.3)$$

where  $z_i = r_i \cos \theta_i$ . This perturbation is of precisely the same form as that due to a uniform electric field of strength  $e/r^2$ . The second-order energy term is then given by  $-\frac{1}{2}\alpha(e/r^2)^2$ , where  $\alpha$  is the electric polarizability of the atom. (In passing we note that a formal expression for  $\alpha$  can be given, but that if available an experimental value for  $\alpha$  could perfectly well be used for present purposes.) The third-order energy term vanishes identically, as can be seen from parity considerations, while the fourth-order energy term is proportional to  $1/r^8$ . We will here ignore this term, though on the basis of some later discussion it will become clear that it will have no effect on those terms in the expansion of  $\tan \eta$  that we will retain.

In the adiabatic approximation, the above  $1/r^4$  energy term plays the role of the potential between the incident positron and the atom. Thus, we have that at large  $r$  the motion of the positron can be described by a wave function  $g(\mathbf{r})$  that satisfies

$$[\nabla_r^2 + k^2 + \beta^2/r^4 + O(1/r^6)]g(\mathbf{r}) = 0, \quad (3.4)$$

and the appropriate boundary conditions, where

$$\beta^2 = (2m/\hbar^2)(\frac{1}{2}\alpha e^2) = \alpha/a_0,$$

where  $a_0$  is the Bohr radius.

The fact that the leading correction term is of order  $1/r^6$  is a consequence of the adiabatic approximation. If, more properly, one does not make this approximation, it can be shown<sup>13</sup> that there is a nonadiabatic correction which goes asymptotically as  $r^{-5}d/dr$ . This term, however, can be shown to give contributions in the expansion of  $\tan \eta(L)$  which have the same energy dependence as the contributions due to the  $1/r^6$  term. Henceforth it will always be understood when we refer to  $1/r^6$  terms that we are including the nonadiabatic contribution as well.

Having briefly summarized the derivation of the effective  $1/r^4$  interaction, we now turn to the basic problem of the present paper, the derivation of a (modified) ERT for the scattering of a charged particle by a polarizable system. The particular case to be treated in this subsection is the scattering of a positron by a neutral spherically symmetric atom. We will proceed in a fashion analogous to that used in Sec. 2, and we will therefore need the asymptotic form  $\Psi^\infty$  of the scattering wave function and the homogeneous differential equation which it satisfies.

The leading terms in the asymptotic expansion of the scattering wave function can be derived exactly as was done by Castellejo, Percival, and Seaton<sup>14</sup> for the scat-

tering of electrons by hydrogen atoms and for scattering energies below excitation, as these authors point out, the derivation can be directly extended to other atoms. Their results remain valid of course under the replacement of an incident electron by an incident positron. As noted above, however, the atom must not have a permanent quadrupole moment, lest there be a dominating  $1/r^3$  term.

We find then on the basis of their work that the asymptotic form of  $\Psi$  for  $r \rightarrow \infty$  is

$$\Psi = \left[ F + \frac{e^2}{r^2} \sum_n' \sum_{i=1}^Z \frac{(z_i)_{n0}}{E_n - E_0} F_n + O(1/r^3) \right] g(\mathbf{r}) \quad (3.5)$$

where the prime on the sum indicates the exclusion of the ground state  $F$  and where  $g(\mathbf{r})$  satisfies Eq. (3.4) for large  $r$  and the appropriate boundary conditions.

Now there is nothing unique about the choice of  $\Psi^\infty$ . It must satisfy the requirement that  $\Psi$  approaches  $\Psi^\infty$  sufficiently rapidly so that the "modified effective range"  $r_{p0}$ , defined in terms of  $\Psi$  and  $\Psi^\infty$ , exists. Thus, while for  $L=0$   $\Psi$  ultimately approaches  $F \sin[kr + \eta(0)]/kr$ , the difference between  $\Psi$  and this function vanishes so slowly at large  $r$  that  $r_{p0}$  would be infinite if  $\Psi^\infty$  were chosen equal to this function. For  $L=0$ , we will choose

$$\Psi^\infty = FM(r)/r, \quad (3.6)$$

where  $M(r)/r$  is the  $L=0$  solution, for all  $r$ , of

$$\left( \frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + \frac{\beta^2}{r^4} + k^2 \right) M(r) = 0. \quad (3.7)$$

[If  $g(\mathbf{r})$  as defined by Eq. (3.4) is decomposed into partial waves, the radial part of the  $L$ th partial wave approaches  $M(r)/r$ .] In line with our previous paper on central potentials,  $M(r)$  is to satisfy the boundary conditions (with  $L=0$ )

$$M(r) \rightarrow \frac{r}{\beta} \left[ \text{si} \left( \frac{\beta}{r} - \frac{1}{2}L\pi \right) + B_k \cos \left( \frac{\beta}{r} - \frac{1}{2}L\pi \right) \right] \quad \text{for } r \rightarrow 0. \quad (3.8)$$

The choice of  $\Psi^\infty$  as given by Eq. (3.6) will lead to a finite  $r_{p0}$  and has the advantage of being the solution of the simple homogeneous differential equation

$$(H_0 + T_r - \frac{1}{2}Z^2e^2\alpha/r^4 - E)\Psi^\infty = 0, \quad (3.9)$$

where  $H_0$  is the target Hamiltonian.  $\Psi$  of course satisfies

$$(H_0 + T_r + H' - E)\Psi = 0, \quad (3.10)$$

where  $H'$  is given by Eq. (3.1). If we now manipulate the equations for  $\Psi$  and for  $\Psi^\infty$  at energies  $E$  and  $E_0$ , as was done in Sec. 2, we derive the identity

$$k^2 \int (\Psi_0^\infty \Psi^\infty - \Psi_0 \Psi) d\tau = \lim_{r \rightarrow 0} (M_0 M' - M M_0') = B_k/\beta - B_0/\beta. \quad (3.11)$$

<sup>13</sup> M. H. Mittleman and K. M. Watson, Phys. Rev. **113**, 198 (1959).

<sup>14</sup> L. Castellejo, I. C. Percival, and M. J. Seaton, Proc. Roy. Soc. (London) **A254**, 259 (1960).

We now have the effective-range expansion,

$$B_k/\beta \approx B_0/\beta + \frac{1}{2}r_{p0}k^2, \quad (3.12)$$

where

$$\frac{1}{2}r_{p0} \equiv \int [(\Psi_0^\infty)^2 - (\Psi_0)^2] d\tau. \quad (3.13)$$

It can now be verified from Eqs. (3.6) and Eq. (3.5) that  $r_{p0}$  is finite. Note incidentally that ERT is here not used directly on  $k \cot\eta$ , but rather on  $B$ . The connection between  $B$  and  $\cot\eta(0)$  then follows from the known properties of the solutions of Eq. (3.7) and is given by Eq. (I-4.3). For convenience, we repeat the  $L=0$  result

$$k \cot\eta(0) = -1/A + (\pi\beta^2/3A^2)k + (4\beta^2/3A)k^2 \ln(1.23\beta k) \\ + (\frac{1}{2}r_{p0} + \frac{1}{3}\pi\beta - \pi\beta^2/3A^2 - \pi^2\beta^4/9A^3)k^2 + \dots, \quad (3.14)$$

where we have combined several of the terms.

For  $L>0$ , the form of the expansion of  $\tan\eta(L)$  for the present problem is *not* identical with that previously derived for a central potential which goes as  $1/r^4$ . The origin of the difference is not that we are here dealing with a compound system rather than with a central potential. The difference is simply due to the fact that the compound system generates an effective long-range interaction which has terms in  $1/r^6$  (and still higher terms) as well as the term in  $1/r^4$  which was all that was assumed for the central potential. If the central potential had these terms, the form of the expansions would be the same, though of course it would be very much more difficult to actually obtain some of the coefficients for the compound system case. We note that even for  $L=0$  the terms in  $1/r^6$  play a role, but they would only change the form of the expansion for terms of higher powers of  $k$  than those which were retained.

More precisely, a definition of  $\Psi^\infty$  similar to that given in Eq. (3.6)—a form which only includes effects of the  $1/r^4$  term—again leads, with no difficulty, to the identity, Eq. (3.11), but if we try to proceed to Eq. (3.12), we find that  $r_{p0}$  is infinite. The infinity is due of course to the neglect of the  $1/r^6$  term. To better understand this, we point out that the formalism previously developed capitalizes on the fact that the solutions with a  $1/r^4$  are known (Mathieu) functions, so that given the ratio  $B$  of two of these, we can write down the expansion of  $\tan\eta(L)$  up through and including terms in  $k^{2L+3}$ . This, however, cannot be correct for  $L>0$  since it can be shown for example that the neglected  $1/r^6$  interaction contributes a term in  $k^4$ . On the other hand, though we will not prove it here, we have no doubt that the results obtained neglecting the  $1/r^6$  interaction are correct up through  $k^3$  even for  $L>0$ . In particular, then, for the scattering of positrons (or electrons) by atoms,  $\tan\eta(L)$  will have the same leading term as for the scattering by a central potential, namely,

$$\tan\eta(L) = \pi\beta^2 k^2 [(2L+3)(2L+1)(2L-1)]^{-1} + \dots \\ \text{for } L \geq 1, \quad (3.15)$$

where the correction is  $O(k^3)$  for  $L=1$  and  $O(k^4)$  for  $L>1$ .

The  $L=1$  case will be considered in more detail in the Appendix. It will there be shown that one can write

$$\tan\eta(1) = \pi\beta^2 k^2 / 15 + \beta^3 k^3 / [9B_0(1)] + O(k^4), \quad (3.16)$$

where  $B_0(1)$  appears in the zero-energy form of Eq. (3.8). [See also Eq. (I-5.1).]

Since it plays no role, the spin of the positron has been entirely neglected. To introduce it—this makes the transition to the electron scattering case easier, for there by virtue of the Pauli principle the spin does play a role—we would have to take a linear combination of ground-state wave functions with different  $z$  projections of the angular momentum of the atom, multiplied by appropriate spin-angle functions.

## B. Incident Particle Indistinguishable

In the scattering of electrons by atoms one must concern oneself with the difficulties that arise from the need to include the Pauli principle and with the difficulties that have their origin in the effective long-range interaction. These difficulties have each been treated, the first in Sec. 2(B) and the second in Sec. 3(A) and no new problems arise when the two difficulties appear simultaneously. Our basic identity, Eq. (3.11), is now

$$B_k/\beta = B_0/\beta + k^2 \int [\sum_i \psi_i^\infty \psi_{i0}^\infty - \Psi_0 \Psi] d\tau, \quad (3.17)$$

with  $\Psi$  and  $\Psi_0$  appropriately symmetrized, and we again have the effective range theory approximation, Eq. (3.12), with Eq. (3.13) replaced by

$$\frac{1}{2}r_{p0} = \int [\sum_i (\psi_{i0}^\infty)^2 - (\Psi_0)^2] d\tau, \quad (3.18)$$

where

$$\psi_{i0}^\infty = P_i(Z+1)^{-1/2} F(-i) X_{\frac{1}{2}} \\ \times [\beta^{-1} \sin(\beta/r_i) - A^{-1} \cos(\beta/r_i)]. \quad (3.19)$$

Equation (3.14) for  $k \cot\eta(0)$  is still valid, but with  $r_{p0}$  as just defined.

The number of phase shifts required for a description of electron-atom scattering will depend upon the total angular momentum  $J$  of the atom and the incident orbital angular momentum  $L$  of the incident electron. For  $L=0$ , for example, there will be one phase shift if  $J=0$  and two phase shifts if  $J \neq 0$ . The situation is slightly more complicated if  $L \neq 0$ . The determination of the number of phase shifts for positron-atom scattering is rather similar, but somewhat simplified, by the fact that the mechanical spin of the positron plays no role whatever. For  $L=0$ , for example, there will be only one phase shift independent of the value of  $J$ .

### C. Expansion about Energy of Bound State

If the incident particle plus the atom can form a bound state with an energy below  $E_0$  by an amount  $\hbar^2\gamma^2/2m$ , the asymptotic form of the bound-state wave function will be that given by Eq. (3.6), but with  $M_k$ , (generally written simply as  $M$ ), replaced by the exponentially decaying function  $M_\gamma$ . [ $M_\gamma$  satisfies Eq. (3.7) with  $k^2$  replaced by  $-\gamma^2$ .] If  $\gamma$  is small and known, it will often be useful for small incident energy to expand about the energy of the bound state rather than, as in Secs. 3(A and B), about zero incident energy. For the expansion about the energy of the bound state we can once again recover the equations found for the center of force, with the effective range appropriately defined.

For later reference, we note in particular that the relationship

$$1/A = \gamma - \frac{1}{2}\rho_\gamma\gamma^2 + O(\gamma^3 \ln\gamma), \quad (3.20)$$

where  $\rho_\gamma$  is defined in the standard way (that is, neglecting polarization), a relationship which was shown<sup>6</sup> to be valid for scattering by a central potential which vanishes as  $1/r^4$ , remains true for electron-atom scattering. (It is to be recalled that  $r_0$  as normally defined does not even exist when there is present a long-range  $1/r^4$  potential, but that due to the decay of the various functions introduced in the standard definition of  $\rho_\gamma$ ,  $\rho_\gamma$  does exist.)

### 4. SCATTERING BY HYDROGEN ATOMS

The low-energy phase shifts for the scattering of electrons by hydrogen atoms are expressed by Eqs. (3.14) and (3.16). Denoting singlet and triplet by the subscripts  $S$  and  $T$ , respectively, the low-energy  $L=0$  scattering is then determined by a knowledge of  $\beta$  and of the four scattering parameters  $A_S$ ,  $A_T$ ,  $r_{p0S}$  or  $\rho_{p\gamma S}$ , and  $r_{p0T}$ . For  $L>0$  the scattering phase shifts are determined, at least to lowest order, by  $\beta$  alone.

$\beta$  can be calculated precisely and has the value  $\beta = (\frac{9}{2})^{1/2}a_0$ . The most reliable values of the scattering lengths are probably those obtained from a rigorous minimum principle.<sup>15</sup> Assuming only that there is one and only one singlet bound state of  $H^-$  and no triplet bound states of  $H^-$ , it was found<sup>16</sup> that

$$A_T \leq 1.91a_0, \quad A_S \leq 6.23a_0.$$

<sup>15</sup> L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959); L. Rosenberg, L. Spruch, and T. F. O'Malley, *ibid.* **118**, 184 (1960).

<sup>16</sup> L. Spruch, L. Rosenberg, and T. F. O'Malley, Phys. Rev. **119**, 164 (1960). The bounds quoted above have recently been superseded by calculations of C. Schwartz [Phys. Rev. **124**, 1468 (1961)] who finds  $A_S \leq 5.965 a_0$  and  $A_T \leq 1.7686 a_0$ . These newer values put a slightly altered emphasis on some of the following discussions. *Added in proof.* We might add that despite their great accuracy, Schwartz's results would probably not have been as ideally suited for the present analysis as one might at first imagine since the zero energy and nonzero energy cases were treated on a different basis, the long range effects on the wave function having been explicitly introduced only at zero energy.

Since the other bound is not known, it is not possible to make any rigorous statements about the accuracy of these results, but they are probably at least roughly correct since they agree reasonably well with results obtained by the use of effective-range theory<sup>17</sup> and with results obtained from numerical analyses<sup>18-20</sup> of the adiabatic approximation. They also lead to consistent results in a dispersion-theoretic analysis.<sup>21</sup>

$\beta$  and the parameters  $A_S$  and  $A_T$  are sufficient to determine the cross section rather well up to perhaps  $\frac{1}{2}$  ev. Unfortunately comparison with experimental results is not possible, for these experiments cannot at this time be performed. It would be interesting to make the comparison for He, where the experiments are relatively simpler and where the theoretical calculations could be performed.

To proceed to energies up to about 1.5 ev, one must know the singlet and triplet effective ranges. A reasonably accurate value of  $\rho_{p\gamma S}$  can be obtained from some recent estimates of  $\rho_{\gamma S}$ , even though these estimates did not explicitly take long-range effects into account. This will be shown shortly. It will further be shown that it is possible to extract an estimate of  $r_{p0T}$ , in the adiabatic approximation, from a published calculation<sup>19</sup> of electron-hydrogen scattering.

Above about 1.5 ev the results of the present paper are not valid because the Mathieu function expansions which we used are valid for  $\beta^2 = (\frac{9}{2})a_0^2$  and for  $L=0$  only up to  $\nu=1$ .<sup>22</sup> As noted previously,<sup>6</sup> this is not an inherent limitation, but the extension to higher energies along the present lines has not been attempted because long-range effects are probably not very important much above 1.5 ev.

The fact that the negative hydrogen ion  $H^-$  has a singlet but apparently not a triplet bound state makes the analysis of the singlet scattering of electrons by hydrogen somewhat simpler than that of triplet scattering. We will therefore treat singlet scattering first.

### A. Singlet Electron Scattering

Effective-range theory was first applied to the scattering of electrons by hydrogen atoms by Borowitz and Greenberg.<sup>23</sup> They used the ERT approximation,

$$1/A_S \approx \gamma - \frac{1}{2}\rho_{\gamma S}\gamma^2, \quad (4.1)$$

<sup>17</sup> T. Ohmura and H. Ohmura, Phys. Rev. **118**, 154 (1960).

<sup>18</sup> M. J. Seaton and J. B. Wallace, Proc. Phys. Soc. (London) **72**, 701 (1958).

<sup>19</sup> A. Temkin and J. C. Lamkin, Phys. Rev. **121**, 788 (1961).

<sup>20</sup> See also Temkin's nonadiabatic results; A. Temkin, Phys. Rev. Letters **6**, 354 (1961); and A. Temkin, Phys. Rev. (to be published). *Added in proof.* These results take the long range  $1/r^4$  effect into account at zero and at nonzero energies, and might therefore seem to be ideally suited for an analysis of the present type. Unfortunately, they are not quite as accurate as the results of Schwartz (see reference 16), especially for singlet scattering.

<sup>21</sup> E. Gerjuoy and N. A. Krall, Phys. Rev. **119**, 705 (1960); N. A. Krall and E. Gerjuoy, *ibid.* **120**, 143 (1960).

<sup>22</sup> This occurs in general when  $\beta^2 k^2 \approx 1/2$ . See reference 6.

<sup>23</sup> S. Borowitz and H. Greenberg, Phys. Rev. **108**, 716 (1957).

the known value of  $\gamma$ , and a variational estimate of  $A_S$  to make an estimate of  $\rho_{\gamma S}$ . With the availability of very accurate  $H^-$  bound-state wave functions,<sup>24</sup> it was recognized<sup>3,17</sup> that Eq. (4.1) could then be utilized in a different and more powerful manner; with  $\gamma$  and  $\rho_{\gamma S}$  obtained from the  $H^-$  wave function, Eq. (4.1) could be used to estimate  $A_S$ . The values<sup>17</sup>  $\gamma=0.23559a_0^{-1}$  and  $\rho_{\gamma S}=2.65$  give  $A_S \approx 6.2a_0$ .

Equation (4.1) was derived under the assumption of short-range potentials whereas the present problem involves long-range potentials. It was noted, however, at the end of Sec. 3 that Eq. (4.1) is valid, to terms in  $\gamma^2$ , even in the presence of the long-range  $1/r^4$  potential. Since we also know<sup>6</sup> [see Eqs. (I-6.9) and (I-6.10)] that

$$\frac{1}{2}\rho_{p\gamma S} + \frac{1}{3}\pi\beta = \frac{1}{2}\rho_{\gamma S} + O(\gamma), \quad (4.2)$$

we have that  $\rho_{p\gamma S} \approx -1.7a_0$  to zeroth order in  $\gamma$ . We also have that  $A_S \approx 6.2a_0$  to terms in  $\gamma^2$ , but this estimate is however less reliable than might at first appear to be the case, for whereas for short-range potentials the corrections would be of order  $\gamma^4$ , the corrections for the present long-range case include  $\gamma^3 \ln \gamma$  and  $\gamma^3$  terms.

Fortunately, it is a relatively simple matter to include the  $\gamma^3 \ln \gamma$  and  $\gamma^3$  terms and thereby obtain an improved estimate of  $A_S$  and of  $\rho_{p\gamma S}$ . Thus, while the coefficient of the  $\gamma^4$  term in the expansion of  $1/A_S$  involves a new parameter, the coefficients of the  $\gamma^3 \ln \gamma$  and  $\gamma^3$  terms in the expansion of  $1/A_S$  involve only  $\beta$ . To find these coefficients, we need higher terms in the expansion than given in Eq. (I-6.6). By expanding Eq. (I-3.9) for  $k^2$  replaced by  $-\gamma^2$ , we obtain

$$m_{\gamma}^2 e^{i\pi} = \beta\gamma \left\{ 1 - \frac{4}{3}(\beta\gamma)^2 \ln\left(\frac{1}{4}\beta\gamma\right) - (20/9)[1 - (6/5)\Psi(3/2)](\beta\gamma)^2 + \dots \right\}. \quad (4.3)$$

Equation (I-6.7) then becomes

$$B_{\gamma} = -\beta\gamma + \frac{1}{3}\pi(\beta\gamma)^2 + \left(\frac{4}{3}\right)(\beta\gamma)^3 \ln\left(\frac{1}{4}\beta\gamma\right) + (20/9)[1 - (6/5)\Psi(3/2)](\beta\gamma)^3 + O(\gamma^4), \quad (4.4)$$

while the expansion for  $\rho_{p\gamma}$  becomes

$$\frac{1}{2}\rho_{p\gamma} + \frac{1}{3}\pi\beta = \frac{1}{2}\rho_{\gamma} - 2\beta^2\gamma \times [\ln\left(\frac{1}{4}\beta\gamma\right) + 2 - 2\Psi(3/2)] + \dots \quad (4.5)$$

If we substitute these two expansions into the  $L=0$  and  $k=0$  form of Eq. (I-6.2),

$$1/A = -B_{\gamma}/\beta - \frac{1}{2}\rho_{p\gamma}\gamma^2 + O(\gamma^4),$$

the resulting approximation to  $1/A$  is

$$1/A = \gamma - \frac{1}{2}\rho_{\gamma}\gamma^2 + \frac{2}{3}\beta^2\gamma^3 \ln(3.35\beta\gamma) + O(\gamma^4). \quad (4.6)$$

When applied to the singlet scattering of an electron by a hydrogen atom, the third term is small compared to the second but is not at all negligible, and changes the estimate from  $A_S \approx 6.2a_0$  as previously quoted to the present estimate of

$$A_S \approx 5.5a_0. \quad (4.7)$$

We also now obtain

$$\frac{1}{2}\rho_{p\gamma S} + \frac{1}{3}\pi\beta \approx 1.00a_0, \quad (4.8)$$

as opposed to the crude estimate of  $1.3a_0$ .

It is extremely difficult to judge the reliability of the estimate of  $A_S$  given by Eq. (4.7). Since  $\gamma$  is small and the successive terms in the series, Eq. (4.6), are decreasing in magnitude, one might perhaps expect the error to be somewhat smaller than the last term. Arbitrarily taking the error to have a magnitude one-half that of the last term gives  $A_S \approx (5.5 \pm 0.4)a_0$ . By virtue of the nature of the argument, a value of  $A_S$  not much below  $6.2a_0$  is certainly not ruled out, but the possibility of a value appreciably below  $6.2a_0$  is suggested. (See also the remarks in reference 16.)

An estimate of the  $L=1$  "scattering length,"  $A(1)$ , will be given in the following subsection.

## B. Triplet Electron Scattering

Of the four low-energy scattering parameters for  $L=0$ , we now have estimates of all but  $\rho_{p0T}$ . The two scattering lengths were determined through the use of a minimum principle and  $\rho_{p0S}$  was obtained from a study of the  $H^-$  bound-state wave function. There is no known minimum principle that can be applied to the determination of  $\rho_{p0T}$  and there is no triplet bound state of  $H^-$  to help us estimate  $\rho_{p0T}$ . It is possible to make a variational estimate of  $\rho_{p0T}$  but we will not do so. Rather we will be content to make a rough estimate of  $\rho_{p0T}$  through the use of the numerical results obtained in the adiabatic approximation. We will also use the numerical data to make some perhaps crude estimates of the parameters which characterize low-energy  $p$ -wave scattering.

Of the calculations that have been made in the adiabatic approximation,<sup>18,19</sup> we will here restrict our attention to that of Temkin and Lamkin. In the evaluation of the perturbation of the ground-state wave function they neglect the possibility that  $r_i$  is larger than  $r$ , and they neglect contributions from other than the dipole term, thereby arriving at Eq. (3.3). In this approximation, the electron-atom interaction contains just one long-range interaction, and this interaction is known exactly. The one-body analysis given previously,<sup>6</sup> as modified by the many-body details discussed in the present paper, is perfectly suited for the analysis of the integro-differential equation which the above authors actually solve numerically. (As we have noted earlier, the situation is slightly more complicated for the real physical problem since that contains additional<sup>18</sup> long-range interactions.) As a check on the accuracy of the numerical calculations and on the validity of the present theory, we will see if Eq. (3.14), with two parameters, can reproduce the numerical values of their  $L=0$  triplet phase shifts. We will at the same time obtain an estimate, in the<sup>18</sup> adiabatic approximation and in the dipole approximation, of  $r_{p0T}$ .

<sup>24</sup> C. L. Pekeris, Phys. Rev. 112, 1649 (1958).



TABLE I. Values of  $\tan\eta(0)/k$  for the triplet scattering of electrons by hydrogen atoms. Row 1 represents the uncorrected results of Temkin and Lamkin, row 2 represents their results corrected to include effects of the long-range interaction beyond  $r=20a_0$ , and row 3 represents the values obtained from Eq. (4.9) with the choice  $A_T=1.69a_0$  and  $r_{p0T}'=-1.7u_0$ . (The latter corresponds to  $r_{p0T}=0.8a_0$ .)

$\tan\eta(0)/k$	0.01	0.05	0.10	0.20	0.30
Uncorrected	-1.90	-1.93	-2.00	-2.18	-2.39
Corrected	-1.74 <sup>a</sup>	-1.87	-1.99	-2.17	-2.39
From Eq. (4.9)	-1.74	-1.87	-1.99	-2.16	-2.26

<sup>a</sup> See reference 20.

It will be preferable to work with the expansion of  $\tan\eta/k$  rather than of  $k \cot\eta$ . The two expansions are of course formally equivalent. However, it was the former expansion that was actually derived, and the inversion to obtain the latter expansion in the form of Eq. (3.14) involves the neglect of higher-order terms which are not in fact negligible because they happen to have rather large coefficients. We have

$$\tan\eta(0)/k = -A - \frac{1}{3}\pi\beta^2k - \frac{4}{3}A\beta^2k^2 \ln(1.23\beta k) - \frac{1}{2}r_{p0T}'A^2k^2 + \frac{1}{3}\pi\beta^2k^3[A^2 + (7\beta^2/117)] + \dots, \quad (4.9)$$

where

$$\frac{1}{2}r_{p0T}' \equiv \frac{1}{2}r_{p0T} + \frac{1}{3}\pi\beta - \frac{1}{3}\pi\beta^3/A^2.$$

In row 1 of Table I, we give the numerical values of  $\tan\eta(0)/k$  for the triplet case as computed by Temkin and Lamkin. These represent the contributions out to  $20a_0$ . The additional contributions from  $20a_0$  to  $\infty$  are not entirely negligible, and row 2 of Table I gives the corrected values. Row 3 gives the values of  $\tan\eta(0)/k$  obtained from Eq. (4.9) with the choice  $A_T=1.69a_0$  and  $r_{p0T}'=-1.7a_0$ ; the latter corresponds to  $r_{p0T}=0.8a_0$ . It is seen that the data are reproduced reasonably well. The results are not too sensitive to the choice of  $r_{p0T}$  so that the value quoted may be somewhat crude.

For  $L=1$  scattering, low-energy scattering is dominated by the long-range potential. The values<sup>25</sup> obtained by these authors for the singlet and triplet cases at  $k=0.1$ , corrected to account for the contribution from  $r>20a_0$ , are  $\tan\eta(1)/(ka_0)^2=0.78$  for the singlet and 1.07 for the triplet. From a comparison with

$$\tan\eta(1)/k^2 = \pi\beta^2/15 - A(1)k + \dots,$$

we find as a crude estimate the results

$$A(1)^T \approx -1.3a_0^3, \quad A(1)^S \approx 1.6a_0^3. \quad (4.10)$$

### C. Positron Scattering

The description of low-energy positron scattering requires only two scattering parameters,  $A$  and  $r_{p0}$ ,

<sup>25</sup> These values are those privately communicated by Temkin, whom we would like to thank.

as opposed to the four needed in electron scattering, for there is no distinction here between singlet and triplet scattering.  $\beta$  is of course the same as for electron scattering and is known. The low-energy scattering is rather more difficult to estimate than for electron scattering since the distortion of the hydrogen wave function is much greater. (The origin of the distortion is apparently the large probability of virtual positronium formation.)<sup>26</sup> Nothing is known about  $r_{p0}$ . Under the very reasonable assumption that the positron cannot be bound to the hydrogen atom, it has been shown<sup>26</sup> that  $A \leq -1.44a_0$ .<sup>27</sup>

### 5. DISCUSSION

We would like to make two comments on the range of validity of the results of the present paper. The first comment is with regard to the result obtained by Casimir and Polder<sup>28</sup> who showed that if retardation effects are properly taken into account, the long-range interaction between two neutral atoms is no longer the Van der Waals'  $1/r^6$  law, but for sufficiently large  $r$  approaches a  $1/r^7$  law. This rather surprising result might suggest that at sufficiently large  $r$  the  $1/r^4$  interaction, in the adiabatic approximation, of an electron with an atom might become perhaps a  $1/r^5$  interaction when retardation effects are taken into account. B. Rosen and S. Borowitz (unpublished) briefly considered this matter and concluded that such would almost certainly not be the case. They point out that in the atom-atom case there are two fluctuating dipole moments (classically there are two rotating dipole moments) and that the interaction between them, therefore, depends upon the time it takes light to travel from one atom to another. In the electron-atom case, on the other hand, the atom has a nonfluctuating dipole moment, induced by the electron, in addition to its intrinsic fluctuating dipole moment, and the induced dipole-electron interaction is the origin of the  $1/r^4$  interaction; this interaction can therefore clearly be expected to remain a  $1/r^4$  interaction even with retardation effects included. The only possible effects of retardation at the extremely small values of  $v/c$  that we are considering might be an entirely negligible change in the coefficient of  $1/r^4$ . Some of the higher-order terms might be more significantly affected, but we are not here considering them. On the basis of the above remarks, we can therefore safely ignore retardation effects. We would like to thank Dr. Rosen and Dr. Borowitz for having raised the question and for having told us of their conclusions.

<sup>26</sup> L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960).

<sup>27</sup> There are a few calculations at variance with this result in the sense that the results obtained correspond to an effective repulsion between the positron and the H atom, rather than the effective attraction implied by the above negative scattering length. Very recently C. Schwartz, using a very elaborate trial function, found  $A \leq -2.10a_0$ . [C. Schwartz, Phys. Rev. **124**, 1468 (1961).]

<sup>28</sup> H. B. G. Casimir and D. Polder, Phys. Rev. **73**, 360 (1948); H. B. G. Casimir, J. chim. phys. **46**, 407 (1949).

Our second comment has its origin in the fact that even within the domain of nonrelativistic theory, the question of the validity of the adiabatic approximation might seem to be a relevant one. In fact it is not. It is very important to stress that the present results do *not* depend upon the general validity of the adiabatic approximation. Rather, all that is demanded is that at sufficiently large  $r$  the prediction of the adiabatic approximation, that the effective potential go as  $1/r^4$ , be valid, and this has been shown to be the case.<sup>14</sup>

To further clarify this question, it might be helpful to contrast our situation with that which exists in an actual calculation based on the adiabatic approximation. The results of such a calculation might be very accurate but it can certainly not be exact since the adiabatic approximation is surely not valid everywhere. The results of the present paper, on the contrary, depending as they do only upon the *asymptotic* validity of the adiabatic approximation, *are* exact. On the other hand, the aim of the present paper is very much less ambitious. We obtain not the numerical values of  $\tan\eta(L)$ , but only the form of the expansion of  $\tan\eta(L)$ ; furthermore, while an estimate has been stated, no attempt has been made to truly delineate the range of energy over which the expansion is valid.

We have thus far restricted ourselves to atoms which are spherically symmetric. We would now like to consider very briefly the scattering of electrons (or positrons) by atoms which are not spherically symmetric. (Oxygen is a particularly interesting example.) These atoms will in general have an electric quadrupole moment  $Q$  and the long-range interaction (which arises in *first* order) will therefore go as  $CQe/r^3$ , where the constant  $C$  is of the order of unity, and depends upon the angular momentum projection of the atomic ground state. (Ultimately, one must of course average over the various possible projections if one uses unpolarized targets.) This  $1/r^3$  term must necessarily dominate over the term ( $e^2\alpha/2r^4$ ), but the question as to the value of  $r$  at which this occurs is of some interest. Since a typical value of  $Q$  will be of the order of  $ea_0^2$ , while a typical value of  $\alpha$  will be of the order of  $a_0^3$ , we find that the quadrupole  $1/r^3$  term will dominate over the induced dipole  $1/r^4$  term even at values of  $r$  as small perhaps as  $a_0$ . It may be worth remarking that the cross section due to a potential which vanishes as  $1/r^3$  diverges logarithmically at zero incident energy,<sup>29</sup> though it may become very small even for small energies.

The  $1/r^3$  quadrupole interaction may also be of interest in the scattering of protons by very light nuclei. There the  $1/r^4$  term will be very small because of the small values of nuclear polarizabilities. The difficulties in measuring the effects of the  $1/r^3$  term arise because they would be insignificant at all but very low energies,

<sup>29</sup> The infinity is not very surprising since the Born approximation also gives infinity and this approximation should be expected to be valid since the infinity comes from very large  $r$  where  $V(r)$  is very weak.

and there the effects would probably be almost undetectable because they would be swamped by the Coulomb scattering. We hope nevertheless to examine this case for proton-deuteron scattering.

## APPENDIX

We will consider the  $L=1$  case in more detail. It has been noted that the effective-range derivation with Mathieu functions is not appropriate for the higher partial waves, and a more direct method is called for.<sup>30</sup> Nevertheless, by making certain physically motivated approximations, we can extend the effective-range method to include  $L=1$ . It will turn out that the errors generated by these approximations are of higher order in  $k$  than those terms we keep, and so do not affect the final results at all.

The approximations we propose are twofold. The first is the dipole approximation, implied by Eq. (3.3) *ff*. The second is the adiabatic assumption for the wave function  $\Psi$ , or the neglect of nonadiabatic terms. This is equivalent to writing  $\Psi$  in a product form  $\Psi = F'(\mathbf{r}_1 \cdots \mathbf{r}_z; \mathbf{r})f(\mathbf{r})$  and then letting the kinetic energy operator  $T_r$  commute with  $F'$  in the Schrödinger equation. Both approximations need be made only for very large  $r$ , and can be shown to produce an error in  $\eta(L)$  of order  $k^4$ . (These approximations were not made for  $L=0$ .) We may now choose

$$\Psi^\infty = \left[ F + \frac{e^2 t(\mathbf{r})}{r^2} \sum_n' \sum_{i=1}^z \frac{(z_i)_{n0}}{E_n - E_0} F_n \right] \frac{M(\mathbf{r})}{r}, \quad (\text{A1})$$

where  $t(\mathbf{r}) \rightarrow 1$  as  $r \rightarrow \infty$ , and vanishes sufficiently fast as  $r \rightarrow 0$ , and is smooth but otherwise arbitrary. In the approximation noted above, it follows from Eqs. (2.1) and (3.7) that  $\Psi^\infty$  satisfies the inhomogeneous equation,

$$(H_0 - E + T_r - \frac{1}{2}e^2\alpha/r^4)\Psi^\infty = \frac{e^2 t(\mathbf{r})}{r^2} \times \sum_n \sum_{i=1}^z (z_i)_{n0} F_n \frac{M(\mathbf{r})}{r}. \quad (\text{A2})$$

One then proceeds in the usual way and arrives at the standard identity, Eq. (3.11), the inhomogeneous term having played no role. The significant point is that, in the approximation we have made, the difference at zero energy between  $\Psi_0$  and  $\Psi_0^\infty$  falls off fast enough so that the  $r_{p0}$  defined by Eq. (3.13) is finite.

<sup>30</sup> It is a weakness of the present formalism, relying as it does on a knowledge of the exact solution of Eq. (3.7), that a certain sleight of hand is required to derive the simple result, Eq. (3.15), even though it enables one to derive relatively easily the much more complicated result, Eq. (3.14). A consistent and general approach based on asymptotic expansions is now being investigated by Dr. J. B. Keller and Dr. B. Levy. This approach will at the same time allow one to include, for example, the  $1/r^3$  terms.

Given this expression, Eq. (3.12) for  $B(1)$ , we can now write the expansion of  $\tan\eta(1)$  through terms in  $k^5$ , but since we have in effect neglected terms in  $k^4$ , we will have to be satisfied with Eq. (3.16).

The above discussion is clearly not a proof. We have included it nevertheless because we are rather certain that the result is correct, having looked at the problem along the lines indicated by Keller and Levy.

## Electron Triplet Production by High-Energy Photons in Hydrogen\*

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The 323-Mev hardened bremsstrahlung beam from the Berkeley synchrotron was used to produce electron-positron pairs and triplets in a 4-in.-diam liquid hydrogen bubble chamber. It was found that the experimental triplet cross sections for detectable recoils (momentum greater than 0.27 Mev/c) and for recoils with momentum greater than  $mc$  rise logarithmically with photon energy to 100 Mev, then level off at approximately 2.8 mb and 1.5 mb, respectively. The total triplet cross section agrees with that of Borsellino above 20-Mev photon energy. No contribution due to exchange terms was found. The positron energy distribution agrees with that of Wheeler and Lamb. The recoil momentum distribution agrees substantially with that of Suh and Bethe. Approximately one event due to multiple pair production was expected. None was found.

### I. INTRODUCTION

**E**LECTRON pair production by a photon in the Coulomb field of an electron, commonly called triplet production, is one of the major electromagnetic processes contributing to the absorption of energetic photons in light elements.

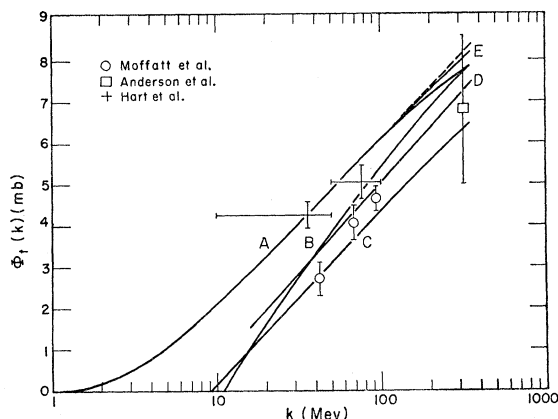


FIG. 1. Results of previous measurements of the total triplet cross section,  $\Phi_t(k)$ , in the energy range of this experiment. The experimental points are those of Anderson *et al.*,<sup>9</sup> Hart *et al.*,<sup>13</sup> and Moffatt *et al.*<sup>10</sup> Also shown are the theoretical cross sections of Watson<sup>8</sup> (curve D), Borsellino<sup>4</sup> (curve B), and Votruba<sup>6</sup> (curve C), corrected to include screening; and the Wheeler-Lamb triplet and Bethe-Heitler [H. A. Bethe and J. Ashkin, in *Experimental Nuclear Physics*, edited by E. Segrè (John Wiley & Sons, Inc., New York, 1953), Vol. I, p. 252.] pair cross sections for hydrogen (curves A and E).

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Bethe and Heitler<sup>1</sup> originally developed the theory of pair production in the nuclear Coulomb field, taking into account screening of this field by atomic electrons through use of the Fermi-Thomas model of the atom. Their method considered only the static nuclear Coulomb field and thereby neglected the effect of retardation on the nuclear Coulomb potential (due to nuclear recoil), which is negligible in the cases of hydrogen and heavier nuclei.

Perrin<sup>2</sup> was the first to point out the possibility of triplet production. He showed that in the laboratory system the threshold energy is  $k=4mc$ ,<sup>2</sup> twice that for pair production, and estimated the cross section to be the same as that for a nucleus with  $Z=1$ . After Perrin, many authors<sup>3-8</sup> have contributed to this work, making a variety of approximations. Table I summarizes some of the details and Fig. 1 shows their results for the total triplet cross section as a function of photon energy.

Wheeler and Lamb<sup>3</sup> developed triplet theory for high-energy photons along the lines of the Bethe-Heitler pair theory, properly taking Coulomb field screening into

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<sup>8</sup> K. M. Watson, Phys. Rev. **72**, 1060 (1947).