In view of the uncertainty in the initial conditions, the value  $21\pm2$  nsec is quoted for the natural lifetime of the  $(3p<sup>5</sup>4s)<sup>3</sup>P<sub>1</sub>$  state of argon. This value can then be compared with the value 10.5 nsec calculated by Knox.<sup>23</sup>

At present, the decay of the  $4p^55s$  multiplet in krypton is being measured. These measurements will allow comparison to the experimental work of Turner' in addition to the values calculated by Dow and Knox.<sup>24</sup> Since preliminary data indicate that the krypton decay is considerably faster than that for argon and that at a given pressure the krypton signal is much larger than the argon signal, the effect of resonance trapping upon the krypton decay will probably be investigated over a broader range of pressure than that reported here for argon. In addition, it is planned that data will be taken for a variety of initial conditions.

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# Positronium Formation in Positron-Hydrogen Scattering\*

MARGARET FULTON FELS AND MARVIN H. MITTLEMANt Lawrence Radiation Laboratory, University of California, Livermore, California (Received 16 May 1966; revised manuscript received 19 June 1967)

A pair of coupled equations describing positron-hydrogen scattering in the energy range where only positronium in its ground state may be formed is solved numerically. The equations, unlike others previously derived, are local to lowest order. The effects of the polarizability of both hydrogen and positronium are included in various ways. The s-wave phase shift at threshold is close to that obtained previously by solution of the nonlocal equations when no polarization is included, and is dramatically improved when polarization of both hydrogen and positronium is included. The positronium formation cross section is about 40 times smaller than the Born approximation. These are the only comparisons with previous work available.

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## INTRODUCTION

'POSITRON —HYDROGEN scattering is of interest as a representative three-body problem. It is uncomplicated by symmetry requirements introduced by the Pauli principle, but does have the complication of the possibility of a rearrangement collision (positronium formation). The importance of the positronium channel even in elastic scattering has been repeatedly emphasized.<sup>1</sup> Massey<sup>2</sup> and co-workers have allowed for this channel by a variational treatment of the problem. They assume a wave function of the form

$$
\Psi(\mathbf{r}_0,\mathbf{r}_1) = \hat{F}(\mathbf{r}_0)\phi(\mathbf{r}_1) + \hat{G}(\frac{1}{2}(\mathbf{r}_0+\mathbf{r}_1))\chi(\left|\mathbf{r}_0-\mathbf{r}_1\right|), \quad (1)
$$

where  $r_0$  is the coordinate of the positron relative to the infinitely massive proton and  $r_1$  is the electron coordinate relative to the proton.  $\phi$  and X are the groundstate wave functions of hydrogen and positronium, respectively. The form (1) is then inserted in the Kohn principle, which is made stationary with respect to small variations of the unknown functions  $\hat{F}$  and  $\hat{G}$ . The result is a pair of integrodifferential equations determining  $\hat{F}$  and  $\hat{G}$ . The boundary conditions are

$$
\lim_{\substack{r_0 \to \infty \\ r_1 \text{ finite}}} \hat{F} = e^{i \, \mathbf{p}_i \cdot \mathbf{r}_0} + f(\hat{r}_0, \hat{p}_i) \frac{e^{i \, \mathbf{p}_i \cdot \mathbf{r}_0}}{r_0},\tag{2a}
$$

gipjF0

$$
\lim_{\substack{|\mathbf{r}_0+\mathbf{r}_1|\to\infty\\|\mathbf{r}_0-\mathbf{r}_1|\text{ finite}}}\hat{G}=g((\mathbf{r}_0+\mathbf{r}_1)/|\mathbf{r}_0+\mathbf{r}_1|,\hat{p}_i)\frac{e^{i\omega_1+\mathbf{r}_1+\mathbf{r}_1/2}}{|\mathbf{r}_0+\mathbf{r}_1|/2}.
$$
 (2b)

Here  $f$  is the elastic-scattering amplitude and  $g$  is the rearranged amplitude. We assume here that the only rearranged channel which is open is the ground-state positronium one. This restricts the incident energy by

$$
\frac{7}{8} > p_i^2 \ge \frac{1}{2},\tag{3}
$$

 $sn$  $l$  ro $+r$  $l$   $l$  2

where  $p_i^2$  is the incident energy of the positron in rydbergs. The  $n=2$  level of hydrogen is energeticalm allowed, but excluded from  $\Psi$  by the choice of the forly (1). The coupled equations described here for  $\tilde{F}$  and  $\tilde{G}$ can be shown to be the lowest order of an exact pair. <sup>3</sup> Higher-order terms modify the potentials occurring in these equations. The higher-order terms represent virtual excitations of both hydrogen and positronium. These higher-order potentials are well known<sup>4</sup> to be

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Rev. 116, 920 (1959).

<sup>&</sup>lt;sup>22</sup> R. S. Knox, Phys. Rev. 110, 375 (1958).

J. D. Dow and R. S. Knox, Phys. Rev. 152, 50 (1966).

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<sup>)</sup>Present address: Space Science Laboratory, University of California, Berkeley, California. ' T.F.O'Malley, L. Rosenberg, and L. Spruch, Phys. Rev. 125,

<sup>1300</sup> (1962).

<sup>\*\*</sup>W. J. Cody, J. Lawson, H. S. W. Massey, and K. Smith, Proc. Roy. Soc. (London), 278, 479 (1964).

nonlocal (integral operators) in this and analogous problems, but the lowest-order terms are only nonlocal in this problem because the coordinates in  $\hat{F}$  and  $\hat{G}$  in (1) are different. This is a geometric complication and can be eliminated by a different choice of coordinates. Chen and Mittleman' have shown how this could be done. They obtain an exact pair of coupled equations analogous to those obtained for  $\hat{F}$  and  $\hat{G}$  which are, in lowest order, local. The essential point of their method is the use of the positron coordinate to label positronium rather than the center-of-mass (c.m.) coordinate as in (1).Since positronium is a body of finite extent and the coordinate used to describe it is not the c.m. , we may expect spurious angular-momentum terms to enter.

The method of Ref. 5 is dependent upon the construction of a projection operator  $P$  such that all the elastic and rearrangement scattering is contained in  $P\Psi$ , where  $\Psi$  is the total wave function. The asymptotic form of  $P\Psi$  is given by

$$
\lim_{\substack{r_0 \to \infty \\ r_1 \text{ finite}}} P\Psi = \left[ e^{i p_i \cdot r_0} + f(\hat{r}_{0j}\hat{p}_i) \frac{e^{i p_i r_0}}{r_0} \right] \phi(r_1), \qquad (4a)
$$
\n
$$
\lim_{\substack{r_0 \to \infty \\ r_0 \to r_1 \text{ finite}}} P\Psi = g(\hat{r}_{0j}\hat{p}_0) \frac{e^{i p_i r_0}}{r_0} \chi(|r_0 - r_1|)
$$
\n
$$
\times \exp i p_i \hat{r}_0 \cdot \left( \frac{r_1 - r_0}{2} \right), \quad (4b)
$$

where

$$
p_f^2 = 2p_i^2 - 1.
$$
 (5)

Chen and Mittleman' chose their projection operator such that

$$
P\Psi = F(\mathbf{r}_0)\phi(r_1) + G(\mathbf{r}_0)\chi(\left|\mathbf{r}_0 - \mathbf{r}_1\right|)
$$
  
× $\exp i\phi_f\phi_0 \cdot (\frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_0))$  (6a)

and obtained equations coupling  $F$  and  $G$ . The asymptotic forms of  $F$  and  $G$  are implied by (4). The exact equations for  $F$  and  $G$  contain effective potentials which in practice must be approximated. The simplest approximation is to neglect all virtual transitions to states not contained in  $\tilde{P}$ . This yields the same equations as the variational method used by Massey with the form (6a) instead of (1). The equations obtained in this way are local.

Polarizability of both hydrogen and positronium are omitted in these equations. These effects may be included by allowing for adiabatic virtual transitions out of the  $P$  part of Hilbert space. We include these by using a potential which gives the correct dipole polarizability but has a phenomenological cutoff at small distances. Various cutoffs are tried.

Clearly, the projection operator implied by (6a) is not unique. It need only be a form which reproduces simply the asymptotic form (4). For instance, the exponential multiplying  $x$  in (6a) could be replaced by

$$
\exp i p_f \hat{r}_0 \cdot (\frac{1}{2} (\mathbf{r}_1 - \mathbf{r}_0)) \beta(r_0), \qquad (6b)
$$

where the function  $\beta$  satisfies  $\beta(\infty) = 1$  but is otherwise unspecified. Inclusion of  $\beta$  will not affect the exact results but when the approximations described in the last paragraph are made,  $\beta$  will then have an effect. The error in the amplitudes can be shown to be linear in the error in the effective potential, and  $\beta$  can be chosen to minimize this error.

The energy range (3) excludes the higher states of positronium. The reason for this was discussed in detail in Ref. 5. Briefly, it is that if such a channel were open, the form  $P\Psi$  [Eq. (6a)], would contain the amplitude for the production of the higher state in G and it would be difficult to extract this amplitude from the amplitude for the ground-state production. This is a result of the lack of orthogonality of the states f, 1s) and f,  $2s$ . The states of hydrogen do not present this problem, since they are othogonal among themselves.

### RESULTING EQUATIONS

We shall merely quote here the relevant results of Ref. 5. The projection operator is given by

$$
P = \frac{\delta(\mathbf{r}_0 - \mathbf{r}_0')}{1 - |\Delta(r_0)|^2} = \left[ |i\rangle\langle i| + |f\rangle\langle f| - \Delta(r_0) |i\rangle\langle f| - \Delta^*(r_0) |f\rangle\langle i| \right], \quad (7)
$$
\nwhere

$$
|i\rangle = \phi_{1s}(r_1),
$$
  
\n
$$
|f\rangle = \chi_{1s}(|\mathbf{r}_0 - \mathbf{r}_1|) \exp{i\phi_f \phi_0 \cdot (\frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_0))},
$$
  
\n
$$
\Delta(r_0) = \langle i | f \rangle = \int d^3r_1 \phi_{1s}(r_1) \chi_{1s}(|\mathbf{r}_0 - \mathbf{r}_1|)
$$
  
\n
$$
\times \exp{i\phi_f \phi_0 \cdot (\frac{1}{2}(\mathbf{r}_1 - \hat{\mathbf{r}}_0))}. \quad (8)
$$

The coupled equations for  $F$  and  $G$  are

$$
[E - \langle i | \mathfrak{F} c | i \rangle] F + [\Delta E - \langle i | \mathfrak{F} c | f \rangle] G = 0, \qquad (9a)
$$

$$
[E - \langle f | \mathcal{R} | f \rangle G + [\Delta^* E - \langle f | \mathcal{R} | i \rangle] F = 0, \qquad (9b)
$$

where the effective Hamiltonian is given by

$$
\mathcal{K} = H + H[Q/(E - QHQ)]H,
$$
  
 
$$
Q = 1 - P.
$$
 (10)

The approximation, in which the coupling to states outside of  $P$  is neglected, is obtained by replacing  $\mathcal X$  with H in (9) (i.e.,  $Q=0$ ). The equations resulting from (9) are still coupled through the kinetic-energy term. This is numerically inconvenient, and a simple algebraic operation decouples them. Next, a partial-wave decomposition of  $\overline{F}$  and  $\overline{G}$ , is made:

$$
F(\mathbf{r}) = \sum_{l=0}^{\infty} i^{l} (2l+1) (1/r) F_{l}(r) P_{l}(\mu) ,
$$
  
(11)  

$$
G(\mathbf{r}) = \sum_{l=0}^{\infty} i^{l} (2l+1) (1/r) G_{l}(r) P_{l}(\mu) ,
$$

where  $\mu = \hat{p}_i \cdot \hat{r}_0$ .

<sup>p</sup> J. C. Y. Chen and M. H. Mittleman, Ann. Phys. (N. Y.) 37, 269 (1966).

The resulting equations are

$$
\left\{p_i^2 + \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{1}{1-|\Delta|^2} \left[-\upsilon_a - \frac{2}{r}(1+r)e^{-2r} - 2\Delta S + \frac{2}{r}|\Delta|^2\right]\right\}F_l + \frac{1}{1-|\Delta|^2}
$$
\n
$$
\times \left\{\Delta\left[\frac{1}{2}(1+p_f^2) + ip_f\frac{d}{dr} + \frac{2p_f^2}{r^2} + \upsilon_b - \frac{2}{r}(1-e^{-r}(1+\frac{1}{2}r))\right] + 2S^* + 2\Delta'd/dr + \Delta''\right\}G_l = 0, \quad (12)
$$
\n
$$
\left\{\frac{d^2}{dr^2} - \frac{l(l+1) + 2p_f^2}{r^2} - ip_f\frac{d}{dr} + \frac{1}{1-|\Delta|^2}\left[\left|\Delta\right|^2\left(-ip_f\frac{d}{dr} - \frac{2p_f^2}{r^2} - p_i^2 + \frac{2}{r}\right) - \Delta^*(\Delta'' + 2\Delta'd/dr) - (2/r)\right.\right.
$$
\n
$$
(1+\frac{1}{2}r)e^{-r} - 2\Delta^*S^* - \upsilon_b\right\}G_l + \frac{1}{1-|\Delta|^2}\left\{2S + \Delta^*\left[\upsilon_a - \frac{2}{r} - \frac{2}{r}(1+r)e^{-2r}\right]\right\}F_l = 0,
$$
\n(13)

where

$$
S(r) = \int d^3r_1\phi_{1s}(r_1)\frac{1}{|\mathbf{r}-\mathbf{r}_1|}\chi_{1s}(|\mathbf{r}-\mathbf{r}_1|) \exp{-ip_f\phi} \cdot (\frac{1}{2}(\mathbf{r}_1-\mathbf{r}))
$$
(14)

and  $\Delta(r)$  is given by (8). The functions  $\mathcal{V}_a$  and  $\mathcal{V}_b$  are the polarization potentials of hydrogen and positronium, respectively. They are taken as zero in the approximation described here. Equation (12) presents no unusual features, but (13) does. Note that the centrifugal term is modified by an energy-dependent term  $(2p_f^2/r^2)$ . The factor 2 is proportional to  $\int d^3r r^2 \chi^2(r)$ , the "size" of positronium. This term results from the fact that an off-center coordinate is used to describe the outgoing positronium atom. The term  $-i p_f d/dr$  is really just the term  $p_f^2$ . It takes this form because the outgoing wave boundary condition Eq. (4b) is built into the projection operator through the presence of the exponential factor in  $| f \rangle$ , Eq. (8). At large distances  $G_l \sim e^{i p_f r}$ , so that  $-i p_f(dG_l/dr) \sim p_f^2G_l$ .

The lowest-order terms of the effective potential are given by expectations of  $\delta H$  between the states  $|i\rangle$  and  $|f\rangle$ , where

$$
\delta H = H[Q(E - QHQ)]H.
$$
 (15) 
$$
\tau_a = -\frac{9}{2}(r^2 + d_a^2)^{-2}
$$

It is clear from the form of  $S$  or  $\Delta$  that the expectation  $\langle i|0|f\rangle$  of any operator  $0(r_0)$  which is bounded as  $r_0 \rightarrow \infty$ will vanish exponentially in this limit. We shall not be interested. in such terms, so only diagonal terms  $\langle i|\delta H|i\rangle$  and  $\langle f|\delta H|f\rangle$  are of any interest. Consider the term  $\bra{i}\delta H\ket{i}$ . In the limit  $r_0\rightarrow\infty$  we use the hydro genic states as the complete set in which we expand the intermediate states of  $\delta H$ . This will involve terms like  $\Delta$  and S, since Q contains  $| f \rangle$ . These may be discarded, since again they vanish exponentially. Therefore,  $P$  in  $Q$  could be replaced by the straightforward projection operator for the scattering of a charged particle on hydrogen with only the ground. state in cluded in P. The term  $\langle i|\delta H|i\rangle$  at large distances, .therefore, is just the polarization potential of hydrogen.

The dominant term is

$$
\mathbb{U}_a(r) \longrightarrow -\frac{9}{2}(1/r^4). \tag{16}
$$

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Similarly,  $\langle f | \delta H | f \rangle$  is the polarization potential of positronium  $\mathbb{U}_b$ , the dominant term of which is

$$
\mathbb{U}_b \to -36/r^4. \tag{17}
$$

Furthermore, the simple scaling relation

$$
\chi_n(r) = \left(\frac{1}{8}\sqrt{8}\right)\phi_n\left(\frac{1}{2}r\right) \tag{18}
$$

yields the approximate result

$$
\mathbb{U}_b(r) = \frac{1}{2} \mathbb{U}_a(\frac{1}{2}r) , \qquad (19)
$$

which we use to determine  $\mathbb{U}_b(r)$ , having chosen  $\mathbb{U}_a(r)$ . Equations (12) and (13) were solved with five different choices of  $\mathcal{V}_a$ . In the first case (I) we take  $\mathcal{V}_a=0$ . In the second (II) we use the Buckingham form,

$$
\mathbb{U}_a = -\frac{9}{2}(r^2 + d_a^2)^{-2},\tag{20}
$$

with  $d_a = 1$ . In the third choice (III) we use (20) with  $d_a=2$ . The final two use

$$
U_a = -\frac{9}{2}\left\{1 - e^{-2x}\left[1 + 2x + 2x^2 + \frac{4}{3}x^3 + \frac{2}{3}x^4 + \frac{4}{27}x^5\right]\right\}1/r^4, \quad (21)
$$

with  $x=r/d_a$ , where in the fourth choice (IV)  $d_a=1$ , and in the fifth (V)  $d_a = 2$ . Form (21) was chosen to coincide with the cutoff function obtained from the polarized orbital method as used in Ref. 2.

For these various choices of the polarization potential, the equations for  $F_l$  and  $G_l$  are integrated by a Runge-Kutta scheme. By a change of variables to elliptical coordinates, the evaluation of both  $\Delta(r)$  and  $S(r)$  is reduced to the computation of a simple one-dimensional



FIG. 1. Elastic cross sections in units of  $\pi a_0^2$  as a function of energy in rydbergs. Solid curves: total cross sections for four forms of the polarization potential [labels correspond to numbers in Eqs. (20) and (21)]. Dashed curves: corresponding contribution from s wave.

integral, of the form

$$
\int \frac{e^{-t}}{t} dt,
$$

where the limits of integration are complex functions of  $p_f$  and r. The integration from  $r=0$  to  $r=\infty$  of the coupled equations is executed in three stages: first, a power-series solution is found for  $r \ll 1$ , enabling one to start the numerical integration at  $0 < r = \epsilon \ll 1$ ; Runge-Kutta integration takes the solutions to a large value of  $r=r_0$ ; and then the long-range effect of the polarization potential, beyond  $r=r_0$ , is calculated by first-order perturbation theory.

The general asymptotic solutions for Eqs. (12) and (13) are given by

$$
F_i(r) \underset{r \to \infty}{\sim} \frac{\sin(p_i r - \frac{1}{2} l \pi)}{p_i} + \beta_1 e^{i p_i r}
$$

and

$$
G_l(r) \underset{r \to \infty}{\sim} \frac{\sin(p_f r - \frac{1}{2} l^* \pi)}{p_f} + \beta_2 e^{i p_f r},
$$

where  $l^*(l^*+1)=l(l+1)+2p_f^2$ . The amplitudes f and g are defined in Eq.  $(4)$ , and expanded as

$$
f = \sum_{l=0}^{\infty} (2l+1) f_l P_l(u) ,
$$
  
\n
$$
g = \sum_{l=0}^{\infty} (2l+1) g_l P_l(u) .
$$
\n(23)

(22)

From Eqs. (4), (6a), and (11), the asymptotic forms of

 $F_l$  and  $G_l$  must be

$$
F_l(r) \sim \frac{\sin(p_i r - \frac{1}{2}l\pi)}{p_i} + f_l e^{i(p_i r - l\pi/2)},
$$
  
\n
$$
G_l(r) \sim g_l e^{i(p_f r - l\pi/2)}.
$$
\n(24)

Two independent sets of initial conditions, determining the amplitude of  $F<sub>i</sub>(0)$  and  $G<sub>i</sub>(0)$ , yield two independent sets, of solutions of  $F_l$  and  $G_l$ . By the appropriate linear combination of the two sets, the plane-wave term in  $G$ , given by  $\alpha_2$  in Eq. (22), is eliminated and the proper asymptotic behavior, Eq. (24), is extracted.

A check on the accuracy of the solutions may be found from the conservation equation for this two-channel system,<sup>6</sup>

Im
$$
(f_l) = p_i |f_l|^2 + \frac{1}{2} p_f |g_l|^2
$$
. (25)

Only when the amplitude of  $f_l$  and  $g_l$  were negligible, with respect to the total amplitudes  $f$  and  $g$ , did the did the two sides of (25) differ by more than  $1\%$ . Hence, the numerical accuracy of the total values  $$ and g is about  $1\%$ .

For a given positron energy  $p_i^2$ , the total cross sections for the elastic and exchange channels, respectively, are given by

$$
\sigma_f = 4\pi \sum_{l=0}^{\infty} (2l+1) |f_l|^2,
$$
  
\n
$$
\sigma_{\theta} = 4\pi \sum_{l=0}^{\infty} (2l+1) |g_l|^2 \frac{p_f}{2p_i}.
$$
\n(26)

Beyond  $l=4$ , the contributions from  $f_l$  and  $g_l^*$  were found to be negligible: hence the summation in this calculation extends from  $l=0$  through  $l=4$ . For each of the five polarization potentials, calculations were made at eight energy values over the range given in  $(3)$ .



FIG. 2. Contribution from  $p$  wave to elastic cross section in unit of  $\pi a_0^2$  as a function of energy in rydbergs.

<sup>6</sup>We have neglected the complex (absorptive) part of the potential which enters in  $(12)$  and  $(13)$  when the  $n=2$  level of hydrogen is energetically possible,  $p_i^2 \geq \frac{3}{4}$ . Consequently, Eq. (25) should be numerically correct even above this threshold.

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#### **RESULTS**

In Ref. 2 the elastic-scattering phase shifts in the range below the positronium-formation threshold  $(p_i^2 < \frac{1}{2})$  were calculated in five different ways. Their method D, which starts from our Eq.  $(1)$  as described in the introduction, may be compared with our nopolarization calculation. The difference between the two is just the difference in coordinates in the positronium channel  $[i.e., the difference between Eqs. (1) and (6)].$ The only point of comparison is at the threshold,  $p_i^2 = \frac{1}{2}$ , where the two calculations overlap. The s-wave phase shift of Ref. 2 extrapolates to about  $-0.29$  at the threshold, while ours yields  $-0.32$ . Probably the best value yet obtained is the variational result of Schwartz,<sup>7</sup> which is about  $-0.05$ . Taking this as the correct result, ours is about  $10\%$  further away than the result of the integral equation. Method E of Ref. 2 includes the polarizability of hydrogen by the polarizedorbital method. Our fourth method includes the polarizability of hydrogen in the same way, but also includes the polarizability of positronium which is eight times as great. Our s-wave phase shift at threshold calculated by this method<sup>8</sup> is  $-0.14$ . Extrapolation of method E of Ref. 2 is difficult because of insufficient data.

The total elastic cross section in units of  $\pi a_0^2$  as well as the  $l=0$  contribution to it are shown in Fig. 1. Method II is not included, since it gives a much larger (and less believable) result for the total and  $l=0$  cross section. Clearly,  $d_a=1$  in the Buckingham form is too



FIG. 3. Positronium formation cross section in units of  $\pi a_0^2$ as a function of energy in rydbergs. Solid curves: total cross sections for four forms of the polarization potential. Dashed curves:  $\n *b*-wave contribution.$ 

<sup>8</sup> Actually, methods II, III, and IV all give essentially the same<br>result for this number.



FIG. 4. Contribution from s wave to positronium formation cross section in units of  $\pi a_0^2$  as a function of energy in rydbergs.

small a cutoff in that it contributes an anomalously large, short-range attractive potential.

The inclusion of the attractive polarizations reduces the elastic cross sections, the reduction being the least in method IV. The  $l=1$  contribution is shown in Fig. 2.<sup>9</sup> Their sensitivity to the form of the polarization is evident.

In Fig. 3 the total positronium formation cross section in units of  $\pi a_0^2$  is again shown for the four methods (excluding II, which is again as much as a factor of 10 higher). The dominant partial-wave contribution is  $l=1$ . This is also shown. The sensitivity to the polarization form is also quite pronounced here. In Fig. 4 the s-wave contribution to the positronium formation cross section is shown. Again, the dependence upon the polarization is evident.

The most startling part of the results on positronium formation is the comparison with previous calculations. Massey and Mohr<sup>10</sup> and Cheshire<sup>11</sup> have each done the same Born-approximations calculation. They agree within 20%. Cheshire<sup>11</sup> has also done an impulseapproximation calculation which is about a factor of 15 higher than the Born result in this range and is probably a poor approximation in this energy range. The Born approximation is poorly defined for rearrangement collisions<sup>12</sup> but the results obtained in Refs. 10 and 11 are probably characteristic of all of the different forms.

One can recover the Born approximation from Eqs. (12) and (13) by setting  $G_l = 0$  and dropping the potential terms in the  $F_l$  part of Eq. (12) and by setting  $\mathfrak{v}_a = 0$ and dropping the potential terms in  $G_l$  and the "centrifugal term"  $-2p_f^2/r^2$  in Eq. (13). We have changed Eq.  $(13)$  in various combinations of the above steps and convinced ourselves that distortion of the incident wave and back-coupling from the  $G$  to  $F$  channels both tend

<sup>&</sup>lt;sup>7</sup> C. Schwartz, Phys. Rev. 124, 1468 (1961).

<sup>&</sup>lt;sup>9</sup> The word "contribution" refers to the value  $4(2l+1)|f_l|^2$ , or

 $4(2l+1)|g_l|^2$ , so that it appears in the appropriate units.<br>
<sup>10</sup> H. S. W. Massey and C. B. O. Mohr, Proc. Phys. Soc.<br>
(London) A67, 695 (1954).

<sup>&</sup>lt;sup>11</sup> I. Cheshire, Proc. Phys. Soc. (London) 83, 227 (1964).<br><sup>12</sup> C. Joachain and M. H. Mittleman, Phys. Rev. **140**, A432  $(1965).$ 

to reduce the positronium amplitude (from the Born result) but that the major reduction comes from the "centrifugal" term  $-2\frac{\partial r^2}{r^2}$ . This term arose from the choice of coordinates  $\lceil$  Eq. (6a) $\rceil$  and the requirements on the wave function at  $r \rightarrow \infty$ . However, the continuation to small  $r$  is certainly not unique. For instance, the modification of the basic form (6a) discussed with reference to (6b) would modify the potential in question with the resulting form  $-2(p_f^2/r^2)\beta^2(r)$ . The asymptotic requirement  $\beta(\infty)=1$  ensures the correct asymptotic form for  $\Psi$ , but setting  $\beta(0)=0$  would turn off this term at short distances. We have chosen the form

$$
\beta = 1 - e^{-ar} \tag{27}
$$

and have rerun the problem with several values of the parameter a. For  $a \geq 2$  there are essentially no changes from the results quoted here. This indicates that our results do not depend critically upon the continuation of long-range effects into the origin. For small values of  $a$ , we drastically modify the short-range terms and the results are changed. The parameter a could be interpreted as a variational parameter, and optimized. This requires further calculation which we hope to report on soon.

No experimental evidence is available for comparison

here. However, there are some data on positron-helius<br>scattering.<sup>13</sup> This is a swarm experiment, and its an scattering.<sup>13</sup> This is a swarm experiment, and its analysis<sup>14</sup> depends upon some assumptions concerning positronium formation. One assumption in particular is that positronium will be formed rapidly when it is energetically possible. H the results of this paper are to be relied upon and if they can be extrapolated to helium, then this assumption will have to be reexamined. For this reason, and for the additional reason that direct positron scattering experiments on helium are now conpositron scattering experiments on helium are now con<br>templated,<sup>15</sup> we propose to apply the method used here to that problem.

Note added in proof. B. Bransden and Z. Jundt have reported on a similar calculation at the Fifth International Conference on the Physics of Electronic and. Atomic Collisions, Leningrad, USSR, 1967 (unpublished), in. which they solved the equations associated with our Eq. (1). Their positronium-formation results are drastically different from ours. In particular they show a pronounced peak in the s-wave results near threshold. The reason for the discrepancy is not clear.  $18$  S. Marder, V. W. Hughes, C. S. Wu, and W. Bennett, Phys.

(1956); R. Drachman, *ibid.* 138, A1582 (1965). <sup>15</sup> W. McGowan (private communication).

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## Precise Theory of the Zeeman Spectrum for Atomic Hydrogen and Deuterium and the Lamb Shift\*

STANLEY J. BRODSKY AND RONALD G. PARSONST Stanford Linear Accelerator Center, Stanford University, Stanford, California (Received 17 April 1967)

In this paper we give a complete and straightforward analysis of the  $n=2$  Zeeman structure which is intrinsically accurate to 1 ppm for determining the Lamb shift from present experiments. This analysis takes into account the current experimental and theoretical knowledge of the atomic Hamiltonian. It is shown that the magnetic part of this Hamiltonian can be taken as that of a free electron and a free nucleus. Radi tive corrections to this assumption are shown to be negligible. The total Hamiltonian can th ized in the  $|F, j, l, m_F\rangle$  representation. Matrix representations of the Hamiltonian are given for all  $n=2$ states of hydrogen and deuterium. We give theoretical predictions for the  $l=1$  hyperfine intervals in hydrogen and deuterium which are accurate to 1O ppm. Values of the Lamb shift calculated from the recent Zeeman level crossings of Robiscoe and Cosens are tabulated.

## I. INTRODUCTION

 $H = n = 2$  Zeeman structure of atomic hydrogen and deuterium has served as a precise testing ground. of quantum electrodynamics. Our knowledge of the Lamb shift, the  $2P_{1/2}$ -2S<sub>1/2</sub> interval, and the fine structure separation, the  $2P_{3/2}$ - $2P_{1/2}$  interval, has been determined from an extrapolation to zero field of

experimental measurements of the atomic spectrum in a nonzero magnetic field. In this paper we calculate in detail an accurate extrapolation of the Zeeman levels. This seems especially important now in view of the discrepancy of the measured and predicted Lamb shift.

The first comprehensive analysis of the precise Zeeman structure theory required to interpret the experimental spectrum was given by Lamb in conjunction with the pioneering experiments performed by

Rev. 103, 1258 (1956).<br><sup>14</sup> W. B. Teutsch and V. W. Hughes, Phys. Rev. 103, 1266

Work supported by the U. S. Atomic Energy Commission. f Present address: Department of Physics, Northeastern University, Boston, Massachusetts.