PHYSICAL REVIEW VOLUME 129, NUMBER 3 1 FEBRUARY 1963

Collisions of Slow Electrons and Positrons with Atomic Hydrogen*

PHILIP G. BURKE†
Lawrence Radiation Laboratory, University of California, Berkeley, California

HARRY M. SCHEY
Lawrence Radiation Laboratory, University of California, Livermore, California

AND

KENNETH SMITH
Argonne National Laboratory, Argonne, Illinois

(Received 13 September 1962)

We investigate the scattering of electrons and positrons by atomic hydrogen for projectile energies in the range from 11.0 to 54.4 eV. We calculate (a) the differential and total cross sections for elastic and inelastic scattering, (b) quantities related to polarization and correlation of electron spins, and (c) the polarization of radiation emitted in various electromagnetic transitions. A close-coupling approximation is used in which the total wave function is expanded in hydrogen eigenstates and only terms corresponding to the $1s$, $2s$, and $2p$ states are retained; the wave function is symmetrized or antisymmetrized explicitly in the case of electron collisions. In positron interactions, positronium formation is neglected. The coupled integro-differential equations that result from the approximate wave function are integrated numerically on an IBM-709 or 7090 computer, subject to standard boundary conditions, to yield the reactance matrix elements in each total spin and total angular-momentum state. In the case of electron scattering, the integral terms are treated by means of an iteration procedure. We find for elastic $1s$-$1s$ electron-hydrogen scattering that the inclusion of the $2p$ state in the close-coupling wave function modifies some partial-wave contributions at lower energies; however, the effect on the total cross section is small. The $1s$-$1s$ cross section has a maximum computed value of about $6\pi a_0^2$ at the second quantum excitation energy, and the differential cross section is strongly peaked in the forward direction. For elastic $2s$-$2s$ scattering of electrons, calculated total cross sections are exceptionally large, attaining values of the order of $400\pi a_0^2$ at 11.00 eV; here, too, the differential cross section is strongly peaked in the forward direction. Our calculated inelastic electron-hydrogen $1s$-$2p$ cross sections are in disagreement with experimental results, sometimes by as much as a factor of two. The calculated cross section reaches a maximum of $1.3\pi a_0^2$ at about 20 eV. The predictions for polarization of photons emitted by hydrogen atoms excited by electron bombardment yield a result that, near the $n=2$ threshold, is a rapidly varying nonmonatomic function of energy; again, over-all agreement with experimental results is poor. We support our belief that these discrepancies probably can not be reconciled by any close-coupling calculation. We also present results for the $1s$-$3p$ excitation cross section calculated with a $1s$-$3p$ close-coupled wave function; there are no experimental data for comparison here but we point out the consequences these results have for $1s$-$2s$ excitations. Our calculated total $1s$-$2s$ excitation cross sections show little difference as a result of including the $2p$ state in the close-coupling wave function. Agreement with experiment is again poor although measurements are subject to possible errors in normalization and we suggest further investigation of normalization procedures. As in the elastic case, the differential $1s$-$2s$ cross section is strongly peaked in the forward direction. Measurements of the spin-flip cross section and our calculation of it are in fair agreement at the $n=2$ threshold. The effect of the $2p$ state on elastic positron-hydrogen scattering is quite pronounced, especially for energies immediately above the $n=2$ threshold. For $1s$-$2s$ excitations by positrons, the same effect is seen, but it manifests itself over a wider energy range. Calculated values of reactance matrix elements are provided in tabular form for electron-hydrogen scattering at six energies above threshold.

I. INTRODUCTION

IN a series of earlier papers[1–5] we have described our investigation of electron- and positron-hydrogen atom collisions. In the present work we continue this program and extend it to higher energies and to processes mainly associated with inelastic scattering, not considered earlier. The results presented cover the range of incident electron and positron energies from 11 to 54.4 eV, a range that lies above the threshold for excitation of the second quantum level of hydrogen at 10.2 eV and, for the most part, also above the ionization threshold at 13.6 eV.

The methods underlying our analysis are given in detail elsewhere[2,3] and we shall only dwell upon them briefly to make this paper reasonably self-contained. Our basic assumption is that an adequate representation of the total wave function can be obtained by use of the so-called close-coupling approximation in which the total wave function is expanded in eigenstates of the hydrogen atom, and only a few low-lying states retained.

---

* This work was performed under auspices of the U. S. Atomic Energy Commission.

† Present address: Theoretical Division, Atomic Energy Research Establishment, Harwell, Berkshire, England.

[1] K. Smith, R. P. McEachran, and P. A. Fraser, Phys. Rev. **125**, 553 (1962); see also K. Smith, Phys. Rev. **120**, 845 (1960); and R. P. McEachran and P. A. Fraser, Can. J. Phys. **38**, 317 (1960).

[2] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).

[3] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 163 (1962).

[4] W. J. Cody, J. Lawson, H. S. W. Massey, and K. Smith (to be published).

[5] P. G. Burke and K. Smith, The Low-Energy Scattering of Electrons and Positrons by Hydrogen Atoms, Rev. Mod. Phys. **34**, 458 (1962).

In the case of electrons the resulting expansion is symmetrized or antisymmetrized explicitly. For positrons we neglect positronium formation.

The wave function obtained in the close-coupling approximation leads to a set of coupled radial-linear integro-differential equations which are solved numerically on an IBM 7090 by means of techniques described in an earlier communication.[2]

Although it is usually difficult to justify the close-coupling approximation *a priori*, some insight into its validity is afforded by comparison both with experiment and other calculations, and by investigation of the effects of including different numbers and different combinations of hydrogen states in the expansion. In addition, the approximation can probably be generalized in a straightforward manner to treat electron and positron collisions with heavier atoms. Thus, the results of our work may have some bearing on other, more complicated collision processes.

In this paper we are concerned only with processes involving transitions among the first, second, and third quantum levels of hydrogen; we have, therefore, restricted our close-coupling expansion to these levels only. Such a program is not unique; with the advent of present day computing facilities, this approach has been taken by other workers[6,7] some of whom take into account the $1s$, $2s$, and $2p$ states of hydrogen in their close-coupling wave functions. The present work is, we think, a logical extension of the earlier work. To begin with, we calculate transitions to and from the third quantum level. Second, we carry out the analysis suggested above, making estimates of the accuracy of our results by calculating with different numbers and different combinations of closely-coupled states. Third, we evaluate the partial-wave contributions up to and including L values of 15 or 16 at the higher energies; this usually insures the convergence of the partial-wave expansion to within the accuracy of the calculation (although in certain cases at higher energies we have had to obtain contributions from higher angular momentum states by an extrapolation procedure to estimate the cross sections accurately.) Fourth, we evaluate quantities of interest at an energy interval fine enough to permit quite accurate interpolations between tabulated values. Finally, we go beyond earlier work in the case of positrons to evaluate certain cross sections in the $1s-2s-2p$ approximation.

By and large, when comparison with experiment is possible, our results accord fairly well with measurement. An outstanding and perplexing exception to this is the poor agreement between certain experimental measurements and our best estimates of the $1s-2s$ and $1s-2p$ excitation cross sections for electrons. It is true that our calculations of these quantities are made with a close-coupling wave function which includes only a limited number of hydrogen states; but our experience with this kind of approximation indicates that the addition of individual higher lying states generally has little effect on excitation cross sections. This fact, in conjunction with the quite large magnitude of the discrepancy, leads us to believe that it cannot reasonably be attributed to the omission of a few higher lying states. Indeed, if the discrepancy is to be ascribed to the calculation rather than to the experimental measurements, we feel it represents an inherent failure of the close-coupling approximation which could only be resolved by taking into account many—perhaps all—hydrogen eigenstates, including the continuum.

Insofar as positron scattering is concerned, our work may also be regarded as an extension of earlier work. Elastic scattering of fast positrons by atomic hydrogen has been calculated by Moiseiwitsch and Williams[8] using a simplification of the second Born approximation, and elastic and inelastic scattering of positrons from the s states of hydrogen have been considered by Smith *et al.*,[9] for incident positron energies below the first hydrogen-excitation threshold. In our present work we include the $2p$ state as well, and calculate above threshold cross sections.

There are, as yet, no data available for positron-hydrogen scattering. Nonetheless, positron scattering is of considerable theoretical interest because the relative importance of various positron effects will be different from the corresponding electron case. For example, the mean static interaction of a positron with an atom is repulsive whereas its long-range polarization is attractive, so that the two effects tend to cancel rather than combine as is the case in electron scattering.

We conclude this section with a brief outline of the contents of the remainder of the paper. In Sec. II we give the relevant theory in a much abbreviated form and also present formulas which are referred to later in the paper. In Sec. III we give our results for electron-hydrogen scattering, and these include (a) elastic $1s-1s$ and $2s-2s$ results, (b) $1s-2s$, $1s-2p$, and $1s-3p$ excitation cross sections, with comments pertaining to the validity of the Born approximation for high angular momentum, (c) polarization of the gamma rays emitted in $1s-2p$ excitations, and (d) differential cross sections and quantities related to spin polarization and correlation. In Sec. IV we discuss our results for positron-hydrogen scattering. Finally, in Sec. V we have a brief

---

[6] P. G. Burke, V. M. Burke, R. McCarroll, and I. C. Percival (to be published); K. Omidvar (private communication). In each of these consideration is limited to total angular momenta of 0 and 1 only.

[7] We have been informed by M. J. Seaton that R. Damburg and R. Peterkop have used the $1s-2s-2p$ close-coupling approximation for $L=0$, 1, 2, 3, 4 for several energies and agreement with the relevant parts of our work is "practically exact." The Damburg-Peterkop work will appear as a Letter to Proc. Phys. Soc. (London) with fuller accounts to be given later in the Journal of Experimental and Theoretical Physics and in the Transactions of the Institute of Physics of the Latvian Academy of Sciences.

[8] B. L. Moiseiwitsch and A. Williams, Proc. Roy. Soc. (London) A **250**, 337 (1959).

[9] K. Smith, W. Miller, and A. Mumford, Proc. Roy. Soc. (London) **76**, 559 (1960).

presentation of calculations that includes the simultaneous coupling of the first, second, and third quantum levels for $L=0$ singlet scattering. Tables of the reaction matrix elements are given in the Appendix.

II. RÉSUMÉ OF THEORY

The theory of the close-coupling approximation is well known and has been given by various authors.[2,3,5] In this section we present a brief résumé of that theory, thus providing a glossary of formulas for later reference.

With the proton regarded as infinitely massive, and, therefore, at rest during the scattering, the total wave function depends only upon the coordinates of the two electrons in the case of electron-hydrogen collisions, and upon the coordinates of the bound electron and the incident positron in the case of positron-hydrogen collisions. In the electron case we write

$$\Psi(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)=\frac{1}{\sqrt{2}}\sum_{\Gamma}\left[\Psi_\Gamma(\mathbf{r}_1\sigma_1\hat{r}_2\sigma_2)\frac{F_\Gamma(r_2)}{r_2}-\Psi_\Gamma(\mathbf{r}_2\sigma_2\hat{r}_1\sigma_1)\frac{F_\Gamma(r_1)}{r_1}\right], \quad (1)$$

where the representation is labeled

$$\Gamma=(nk_nl_1l_2LM_LSM_S)$$

and is diagonal in the total orbital-angular momentum L and the total spin S of the system; n and l_1 are the principal and angular-momentum quantum numbers, respectively, of the bound electron; and l_2 and k_n are the orbital-angular momentum and wave number, respectively, of the scattered electron. For positron scattering, there is no need to antisymmetrize the wave function; the second term in Eq. (1) is, as a consequence, not included.

When the wave function Ψ given by Eq. (1) is used in the standard Kohn-Hulthén variational principle appropriate to this system, there results a set of coupled linear integro-differential equations for the functions F_Γ; these equations were first given by Percival and Seaton.[10] When we neglect positronium formation, the same set of equations, with a change in the sign of the charge of the incident particle and the omission of the exchange terms, also describes positron-hydrogen scattering.

The set of equations thus obtained is solved by techniques fully discussed previously,[2] and we determine the physically significant quantities (cross sections, phase shifts, etc.) by fitting the asymptotic forms of the functions F_Γ to the appropriate spherical Bessel functions modified by an asymptotic expansion. We observe that for those channels above threshold we can write

$$F_{\nu'}{}^{LS}(\nu;r)_{r\to\infty}=\frac{A_{LS}}{k_{n'}{}^{1/2}}\left[\delta_{\nu\nu'}\sin(k_{n'}r-\tfrac{1}{2}l_2'\pi)+R_{\nu\nu'}{}^{LS}\cos(k_{n'}r-\tfrac{1}{2}l_2'\pi)\right], \quad (2)$$

where the channel label $\nu\equiv nl_1l_2$ and initial-state quantities are denoted by primes. If there are N channels above threshold, then the submatrix $R_{\nu\nu'}{}^{LS}$ corresponding to given L and S values, is of dimension $N\times N$.

The S matrix describing the scattering can be expressed in terms of the reactance matrix R through the equation

$$S=(1+iR)/(1-iR), \quad (3)$$

and the transition matrix T is given by

$$T=S-1. \quad (4)$$

Finally, the total cross section for a transition $n'l_1'$ to nl_1 is

$$Q(n'l_1'\to nl_1)=\sum_{SLl_2l_2'}\frac{(2L+1)(2S+1)}{4k_{n'}{}^2(2l_1'+1)}|T_{\nu\nu'}{}^{LS}|^2. \quad (5)$$

An observable of importance in this work is the cross section for excitation of a particular p-state magnetic quantum level (npm_1), where m_1 denotes the quantum number of the z component of the bound electron's orbital-angular momentum. Percival and Seaton have shown that this cross section is simply related to P, the fractional polarization of the radiation emitted when the atom decays from the npm_1 level to one of lower energy.[11] For Lyman-α radiation (which is important in the measurement of the cross section for $1s-2p$ transitions) P has been determined experimentally.[12] According to Percival and Seaton, for Lyman-α radiation excited by electron impact, the polarization of the radiation emitted at right angles to the incident electron beam is given by

$$P=3(1-x)/(7+11x), \quad (6)$$

where

$$x=Q(1s\to 2p,\ m=\pm 1)/Q(1s\to 2p,\ m=0).$$

The cross section $Q_\perp(1s\to 2p)$, obtained by counting photons perpendicular to the electron beam and by assuming an isotropic photon distribution, can then be written as

$$Q_\perp(1s\to 2p)=0.918Q+0.246Q(0), \quad (7)$$

where Q is the total cross section and

$$Q(0)\equiv Q(1s\to 2p,\ m=0).$$

Finally, it can easily be shown that in either spin

---

[10] I. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. **53**, 654 (1957).

[11] I. Percival and M. J. Seaton, Phil. Trans. Roy. Soc. (London) A **251**, 113 (1958).

[12] W. L. Fite and R. T. Brackmann, Phys. Rev. **112**, 1151 (1958).

state S,

$$\begin{aligned} Q^S(n's\rightarrow npm) &= (1/k_{n'}^2) \\ &\times \textstyle\sum_{lLL'} [(2L+1)(2L'+1)]^{1/2} T_{npl;n'sL}{}^{LS} \\ &\times T_{npl;n'sL'}{}^{L'S*} C_{1l}(L,0;m_1-m) \\ &\times C_{1l}(L',0;m_1-m), \quad (8) \end{aligned}$$

where the C's are Clebsch-Gordan coefficients in the notation of Blatt and Weisskopf.[13]

At the threshold for excitation, the final-state wave number is zero and thus only the value $l_2=0$ is allowed. It then follows from angular-momentum conservation that only the cross section with $m=0$ in Eq. (8) is nonzero, and, therefore, $x=0$ in Eq. (6). This gives $P=3/7$ at threshold. On the other hand, for very large energies, P approaches zero since x tends to unity in this limit.

In general, the expression for the differential cross section is a complicated one. If, however, we restrict our considerations to the excitation of hydrogen s states from the ground state, the formula simplifies considerably and we have for the scattering amplitude

$$A_{n's,ns}{}^S(\theta) = (1/2ik_{n'}) \textstyle\sum_l (2l+1) T_{n'l,nsl}{}^{lS} P_l(\cos\theta). \quad (9)$$

With $S=0$ the above expression is the singlet scattering amplitude, and with $S=1$, it is the triplet amplitude. In conformity with the notation of Burke and Schey we shall designate these as $G(\theta)$ and $F(\theta)$, respectively.[3] The differential cross section is then given by the standard equation

$$\sigma(\theta)=\tfrac{1}{4}[3|F(\theta)|^2+|G(\theta)|^2]. \quad (10)$$

For positron-hydrogen scattering, the singlet and triplet amplitudes are identical (since there is no exchange). Consequently, a measurement of the differential cross section at each energy exhausts the experimental possibilities and determines the scattering amplitude through Eq. (10) to within a phase factor. For electron-hydrogen scattering, however, there are possibilities of spin changes during the collision, and other quantities in addition to, and independent of, the differential cross section may be measured. This corresponds to the fact that, at low energies, the singlet and triplet amplitudes are, in general, not equal in electron-hydrogen scattering.[2] This problem has been treated in detail elsewhere[3] and we here merely reproduce the relevant formulas. It is found that the quantities of physical interest (cross sections, spin polarizations, and correlations) can be expressed most readily in terms of the five real functions

$$\begin{aligned} k(\theta)&=\tfrac{1}{4}[3F(\theta)F^*(\theta)+G(\theta)G^*(\theta)], \\ m(\theta)&=\tfrac{1}{4}[F(\theta)F^*(\theta)-G(\theta)G^*(\theta)], \\ n(\theta)&=\tfrac{1}{4}[2F(\theta)F^*(\theta)+F(\theta)G^*(\theta)+F^*(\theta)G(\theta)], \quad (11) \\ p(\theta)&=\tfrac{1}{4}[2F(\theta)F^*(\theta)-F(\theta)G^*(\theta)-F^*(\theta)G(\theta)], \end{aligned}$$

and

$$q(\theta)=\tfrac{1}{4}i[F^*(\theta)G(\theta)-F(\theta)G^*(\theta)].$$

Thus, the components of the spin polarizations $\vec{P}$ and the elements of the correlation tensor Q after scattering (denoted by primes) can be related to their counterparts before scattering (unprimed) by

$$\sigma(\theta)P_k{}^{(1)}(\theta)'=n(\theta)P_k{}^{(1)}+p(\theta)P_k{}^{(2)}+q(\theta)\textstyle\sum_{ij}\epsilon_{ijk}Q_{ij},$$

$$\sigma(\theta)P_k{}^{(2)}(\theta)'=p(\theta)P_k{}^{(1)}+n(\theta)P_k{}^{(2)}-q(\theta)\textstyle\sum_{ij}\epsilon_{ijk}Q_{ij},$$

and (12)

$$\begin{aligned} \sigma(\theta)Q_{ij}(\theta)'&=m(\theta)\delta_{ij}[1-\textstyle\sum_l Q_{ll}]+n(\theta)Q_{ij}+p(\theta)Q_{ji} \\ &\quad -q(\theta)\textstyle\sum_k \epsilon_{ijk}[P_k{}^{(1)}-P_k{}^{(2)}], \end{aligned}$$

where

$$\sigma(\theta)=k(\theta)+m(\theta)\textstyle\sum_l Q_{ll}.$$

The subscripts i, j, k, and l each run over the values 1, 2, and 3 corresponding to the x, y, and z directions.

Of these quantities, perhaps the most easily measurable, apart from the differential cross section, are the depolarization ratio $d(\theta)$ and the spin-flip cross section. These are defined by

$$d(\theta)=P_k{}^{(2)}(\theta)'/P_k{}^{(2)}=n(\theta)/\sigma(\theta), \quad (13)$$

and

$$\sigma_{SF}(\theta)=\tfrac{1}{4}|F(\theta)-G(\theta)|^2=\sigma(\theta)[1-d(\theta)]. \quad (14)$$

In later sections we present values of the foregoing quantities for several reactions calculated in the close-coupling approximation.

Lastly, the "exchange cross section," defined by Lichten and Schultz,[14] is $\frac{1}{2}\sigma_{SF}(\theta)$ in the notation of Eq. (14).

III. ELASTIC AND INELASTIC SCATTERING OF ELECTRONS BY ATOMIC HYDROGEN

A. Elastic Scattering

This section deals with our results for two distinct elastic electron-hydrogen collision processes. The first, the more usual, is that in which the target hydrogen atom is in its ground ($1s$) state both before and after scattering; in the second, the target is in the $2s$ state both before and after scattering.

In Table I we list our results for the $1s-1s$ cross section calculated in the $1s-2s-2p$ close-coupling approximation for electron energies from 11.0 to 54.4 eV. Included for comparison are the results for the same process calculated in the $1s-2s$ close-coupling approximation. In both cases we list the individual partial-wave contributions as well as the total cross section, which is given in the column designated "Sum." The values given in Table I indicate clearly that including the $2p$ state significantly modifies partial-wave contributions for $L\geqslant 1$ at lower energies. The fact that the $2p$ state has its major effect on higher partial waves leads us to conclude that the differences between the

---

[13] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, New York, 1952).

[14] W. Lichten and S. Schultz, Phys. Rev. **116**, 1132 (1959).

TABLE I. Partial-wave contributions to the total $1s-1s$ cross section in units of πa_0^2 as calculated in $1s-2s$ close-coupling approximations (rows "a") and in $1s-2s-2p$ close-coupling approximations (rows "b"). Numbers obtained in Born approximation are indicated by parentheses. "Sum" column is the total of all significant partial-wave contributions. All numbers include spin-weighing factors. k^2 is given in atomic units (au).

k^2(au)	Spin \ L		0	1	2	3	4	5	6	7	8	9	Sum
0.81	Singlet	a	0.436	0.046									
		b	0.4474	0.0098	0.0470	≈0.007	0.0013	0.0004					0.513
	Triplet	a	3.687	1.377									
		b	3.6866	1.7307	0.0861	0.0187	0.0040	0.0013					5.527
1.0	Singlet	a	0.286	0.0333	0.0014								
		b	0.2635	0.0101	0.0654	0.0081	0.0019	0.0006	0.0003	0.0001	0.0001	0	0.350
	Triplet	a	2.895	1.157	0.057								
		b	2.9062	1.3720	0.0934	0.0168	0.0059	0.0019	0.0008	0.0004	0.0002	0.0001	4.398
1.21	Singlet	a	0.186										
		b	0.1722	0.0133	0.0580	0.0102	0.0025	0.0009	0.0004	0.0002	0.0001	0	0.258
	Triplet	a	2.297										
		b	2.2973	1.0862	0.0948	0.0160	0.0068	0.0026	0.0011	0.0005	0.0003	0.0001	3.506
1.44	Singlet	a	0.140	0.0107	0.0005								
		b	0.1269	0.0105	0.0351	0.0100	0.0028	0.0011	0.0005	0	0	0	0.187
	Triplet	a	1.829	0.815	0.068								
		b	1.8266	0.8853	0.0938	0.0153	0.0069	0.0031	0.0014	0	0	0	2.832
2.25	Singlet	a	0.088	0.0012									
		b	0.0836	0.0020	0.0049	0.0039	0.0022	0.0011	0.0006	(0.00006)	(0.00002)	(0.00001)	0.098
	Triplet	a	0.971	0.486	0.0718								
		b	0.9657	0.5148	0.0843	0.0143	0.0053	0.0029	0.0016	(0.00017)	(0.00007)	(0.00003)	1.589
4.0	Singlet	a	0.065										
		b	0.0579	0.0089	0.0014	0.0008	0.0007	0.0005	0.0004	0.0002	(0.00009)	(0.00005)	0.071
	Triplet	a	0.412										
		b	0.3979	0.2412	0.0631	0.0140	0.0040	0.0018	0.0011	0.0007	(0.00026)	(0.00026)	0.724

two approximations, the $1s-2s$ and the $1s-2s-2p$, can probably be accounted for in terms of the long-range distortion effects allowed for by the inclusion of the $2p$ state. Our results also indicate, however, that the major part of the total cross section at the lower energies comes from the $L=0$ contribution which is little affected by the inclusion of the $2p$ state; the over-all effect of the $2p$ state is thus relatively small. This suggests that once the $2p$ state has been included in the close-coupling expansion, the inclusion of additional individual higher lying hydrogen states would scarcely change the results, a conclusion we have been able to draw in other phases of our work.[2]

There are, unfortunately, no $1s-1s$ measurements available at the energies considered here and so the question of the accuracy of our calculation, judged on the basis of comparison with experiment, must be left open for the present.

In Table II, we give our $1s-2s-2p$ results for the $2s-2s$ cross section; both the individual partial-wave contributions and the total cross sections are shown. In certain cases our results are supplemented with values calculated in the Born approximation[15]; these are indicated in parentheses. The extended size of the target atom in the $2s$ state can be seen to produce exceptionally large cross sections, particularly at the lower energies.

The values listed in Table II make it clear that at lower energies the calculation has not been carried far enough to achieve convergence in the partial-wave expansion. At the three lower energies, therefore, we give, in addition to the sum of the calculated partial-wave contributions, estimates obtained by assuming that the partial-wave cross sections depend upon the total angular momentum through the relation $\sigma_L \sim \exp(-L/L_0)$, where the constant L_0 is determined by fitting to our calculated results at lower L values. This assumption is borne out well by the higher partial-wave cross sections calculated in our close-coupling approximation (Table II).

B. The $1s-2p$ and $1s-3p$ Excitation Cross Sections

In addition to the elastic processes discussed in Sec. IIIA we have applied close-coupling methods to certain inelastic reactions. In this section we present our results for the $1s-2p$ and $1s-3p$ excitation cross sections.

Our computations for the $1s-2p$ excitations are summarized in Table III; row (a) gives the contributions of the individual total angular-momentum states (spin statistical factors of $\frac{1}{4}$ and $\frac{3}{4}$ are included). For some of the higher angular momenta, we have used results obtained from a Born approximation calculation made by Seaton *et al.*,[15] and such values are designated in the table by parentheses. Since Born results are available, even for small values of L, we are able to compare them with those coming from our close-coupling approximation; for L values greater than six

---

[15] M. J. Seaton, Proc. Phys. Soc. (London) 77, 174 (1961); M. J. Seaton, *ibid.* 77, 184 (1961); J. Lawson, W. Lawson, and M. J. Seaton, *ibid.* 77, 192 (1961); and V. M. Burke and M. J. Seaton, *ibid.* 77, 199 (1961).

TABLE II. Partial-wave contributions to total $2s-2s$ cross section in units of πa_0^2 as calculated in $1s-2s-2p$ close-coupling approximation. Numbers obtained in Born approximation are indicated by parentheses. "Sum" column is the total of all calculated partial-wave contributions. The "Est." column is total of all significant partial-wave contributions, including values (not shown) obtained by extrapolation (see text). All numbers include spin-weighting factors.

k^2 (au)	Spin \ L	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Sum	Est.
0.81	Singlet	7.8183	14.697	22.204	≈20.3	11.069	8.5347											≈84.6	116
	Triplet	16.236	1.1596	90.320	20.372	32.191	25.548											185.83	267
1.0	Singlet	0.2876	0.6943	3.1518	4.3353	2.9037	2.0602	1.4582	1.0806	0.8061	0.6087	0.4670						17.853	19.2
	Triplet	6.2512	17.219	30.629	12.943	5.5748	5.4025	4.3746	3.2417	2.4184	1.8261	1.4010						91.281	95.3
1.21	Singlet	0.0654	1.0493	2.4570	1.8799	1.4780	1.0946	0.7460	0.5693	0.4312	0.3290	0.2540	0.1988					10.553	11.1
	Triplet	2.3015	12.867	14.402	7.9208	3.0248	2.4566	2.2380	1.7079	1.2935	0.9871	0.7620	0.5965					50.558	52.3
1.44	Singlet	0.1665	1.0828	2.1036	0.9919	0.8261	0.6585	0.5032	(0.3783)	(0.2900)	(0.2225)	(0.1723)	(0.1351)	(0.1076)	(0.0868)			7.7252	
	Triplet	1.7193	9.1722	8.9735	5.3636	2.3675	1.5181	1.2407	(1.1348)	(0.8700)	(0.6675)	(0.5169)	(0.4054)	(0.3227)	(0.2604)			34.533	
2.25	Singlet	0.3737	1.0734	1.1929	0.7173	0.3900	0.2481	0.1813	(0.1289)	(0.1062)	(0.0872)	(0.0714)	(0.0582)	(0.0476)	0.0383	0.0315		4.7461	
	Triplet	1.3909	4.1917	3.8692	2.6697	1.5747	0.8993	0.5631	(0.3868)	(0.3187)	(0.2617)	(0.2142)	(0.1745)	(0.1427)	0.1150	0.0946		16.867	
4.0	Singlet	0.2412	0.4968	0.5110	0.4105	0.2911	0.1919	0.1237	0.0809	(0.0495)	(0.0363)	(0.0280)	(0.0225)	(0.0185)	0.0158	0.0133	0.0112	2.5424	
	Triplet	0.7894	1.6547	1.5969	1.2829	0.9436	0.6492	0.4299	0.2815	(0.1484)	(0.1088)	(0.0839)	(0.0674)	(0.0556)	0.0475	0.0399	0.0337	8.2135	

TABLE III. (a) Partial-wave contributions to total $1s-2p$ excitation cross section in units of πa_0^2 calculated in the $1s-2s-2p$ close-coupling approximation. (b) Partial-wave contributions to total $1s-3p$ excitation cross section in units of πa_0^2 calculated in the $1s-3p$ close-coupling approximation. Values obtained in Born approximation are indicated by parentheses. "Sum" column is the total of all significant partial-wave contributions. All numbers include spin-weighting factors.

k^2 (au)	Spin \ L	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Sum
0.81	Singlet a	0.0384	0.0754	0.1095	≈0.010	0.0030	0											≈0.234
	b																	
	Triplet a	0.0007	0.0657	0.0083	0.0505	0.0013	0.0001											0.1265
	b																	
1.00	Singlet a	0.0360	0.1105	0.2532	0.0352	0.0098	0.0025	0.0007	0.0002	0								0.4481
	b	0.0036	0.0152	0.1415	0.0431	0.0013	0	0										0.2047
	Triplet a	0.0033	0.0798	0.0458	0.1671	0.0438	0.0093	0.0020	0.0005	0.0001								0.3518
	b	0.0001	0.0429	0.0001	0.0454	0.0049	0.0002	0.0001										0.0937
1.21	Singlet a	0.0359	0.1105	0.3404	0.0863	0.0301	0.0112	0.0044	0.0016	0.0006	0.0002	0.0001						0.6212
	b	0.0059	0.0086	0.1376	0.0468	0.0122	0.0025	0.0004	0.0001	0								0.2141
	Triplet a	0.0068	0.0629	0.0549	0.1831	0.1046	0.0388	0.0133	0.0050	0.0019	0.0007	0.0003						0.4727
	b	0.0004	0.0209	0.0006	0.0485	0.0260	0.0067	0.0014	0.0002	0								0.1047
1.44	Singlet a	0.0343	0.0815	0.2895	0.1256	0.0508	0.0229	0.0108	(0.0049)	(0.0024)	(0.0012)	(0.0006)	(0.0003)	(0.0001)	(0.0001)			0.6243
	b	0.0025	0 0074	0.0773	0.0468	0.0180	0.0064	0.0021	0.0007	0.0002	0.0001	0						0.1615
	Triplet a	0.0095	0.0416	0.0539	0.1740	0.1404	0.0732	0.0347	(0.0147)	(0.0072)	(0.0035)	(0.0017)	(0.0008)	(0.0004)	(0.0002)			0.5558
	b	0.0007	0.0104	0.0014	0.0392	0.0367	0.0168	0.0061	0.0020	0.0006	0.0002	0.0001						0.1142
2.25	Singlet a	0.0171	0.0176	0.0942	0.0999	0.0695	0.0451	0.0292	(0.0181)	(0.0124)	(0.0084)	(0.0056)	(0.0038)	(0.0025)	0.0016	0.0011	≈0.0007	0.4275
	b	0.0004	0.0031	0.0191	0.0240	0.0181	0.0116	0.0069	0.0040	0.0023	0.0013	0.0007	0.0004	0.0002	0.0001	0.0001	0	0.0923
	Triplet a	0.0106	0.0133	0.0357	0.1077	0.1342	0.1148	0.0838	(0.0542)	(0.0371)	(0.0251)	(0.0169)	(0.0113)	(0.0075)	0.0049	0.0033	≈0.0023	0.6636
	b	0.0008	0.0016	0.0024	0.0196	0.0303	0.0270	0.0189	0.0118	0.0069	0.0039	0.0021	0.0012	0.0007	0.0004	0.0002	0.0001	0.1279
4.00	Singlet a	0.0035	0.0024	0.0169	0.0302	0.0347	0.0329	0.0286	0.0237	(0.0185)	(0.0154)	(0.0127)	(0.0104)	(0.0084)	0.0066	0.0054	0.0044	0.2640
	b	0.0001	0.0006	0.0033	0.0065	0.0078	0.0075	0.0064	0.0051	0.0039	0.0030	0.0023	0.0017	0.0013	0.0010	0.0007	0.0006	0.0535
	Triplet a	0.0052	0.0038	0.0139	0.0394	0.0624	0.0728	0.0719	0.0647	(0.0556)	(0.0463)	(0.0381)	(0.0311)	(0.0252)	0.0199	0.0162	0.0131	0.6076
	b	0.0003	0.0002	0.0015	0.0068	0.0126	0.0156	0.0157	0.0138	0.0117	0.0091	0.0069	0.0052	0.0039	0.0029	0.0022	0.0017	0.1152

TABLE IV. The $1s-2p$ results for $Q(\pm)$, $Q(0)$, and $Q_\perp$, and for polarization of emitted radiation. All numbers include spin-weighting factors.

	Singlet			Triplet			Total results				Polarization
k^2 (au)	$Q(\pm)$	$Q(0)$	Q_{Tot}	$Q(\pm)$	$Q(0)$	Q_{Tot}	$Q(\pm)$	$Q(0)$	Q	$Q_\perp$	P
0.81	≈0.053	≈0.127	≈0.234	0.0149	0.0967	0.1265	≈0.068	≈0.223	≈0.360	≈0.385	≈0.209
1.00	0.0735	0.3011	0.4481	0.0262	0.2994	0.3518	0.0997	0.6005	0.7999	0.8820	0.2835
1.21	0.0913	0.4386	0.6212	0.0482	0.3763	0.4727	0.1395	0.8149	1.0939	1.2047	0.2799
1.44	0.0878	0.4487	0.6243	0.0753	0.4052	0.5558	0.1631	0.8539	1.1801	1.2934	0.2667
2.25	0.0871	0.2533	0.4275	0.1373	0.3890	0.6636	0.2244	0.6423	1.0911	1.1596	0.1800
4.00	0.0740	0.1160	0.2640	0.1654	0.2768	0.6076	0.2394	0.3928	0.8716	0.8968	0.0855

or seven, the two sets of numbers differ by less than a few percent, and we therefore have confidence in the Born approximation for higher L's. At higher energies, partial-wave results are not available for $L>15$ and the entries in the sum column of Table III in such cases are estimates of the converged cross sections obtained by the extrapolation procedure described in Sec. IIIA.

Experimental results, which may be used for comparison, are not given directly in terms of Q, the total cross section, but rather in terms of $Q(+)$, $Q(-)$, and $Q(0)$, which are cross sections for the excitation of the $2p$ state of hydrogen with the magnetic quantum number equal, respectively, to 1, -1, and 0. In the experiments of Fite and Brackmann[12] and of Fite, Stebbings, and Brackmann[16] photons that result from the decay of the hydrogen-atom target to the ground state are observed in a direction perpendicular to the incident electron beam; an average over all directions is then made by assuming an isotropic photon distribution. The resulting quantity, $Q_\perp$, is expressed in terms of $Q(0)$ and $Q=Q(+)+Q(-)+Q(0)$ through Eq. (7). Our close-coupling results for $Q(\pm)$ and $Q(0)$ and the resulting $Q_\perp$ are given in Table IV where the polarization P of the emitted photons calculated by using Eq. (6) is also presented. A comparison of calculated and measured values of $Q_\perp$ is shown in Fig. 1. Agreement is poor; at low energies the close-coupling results are greater than those of experiment by more than a factor of two, and the over-all shape of the two curves is quite different. Figure 1 also shows the Seaton-Born approximation results which agree remarkably well with our close-coupling curve. We are inclined to regard this agreement as largely fortuitous. A comparison of individual R-matrix elements calculated in the Born approximation and in the close-coupling approximation shows that, except for higher L values and energies, the two sets of numbers bear little resemblance to one another; there are frequent discrepancies both in magnitude and sign. However, when the various partial-wave contributions are added to give the total cross section the discrepancies evidently compensate enough to give the agreement we find between the Born results and our own close-coupling cross section.

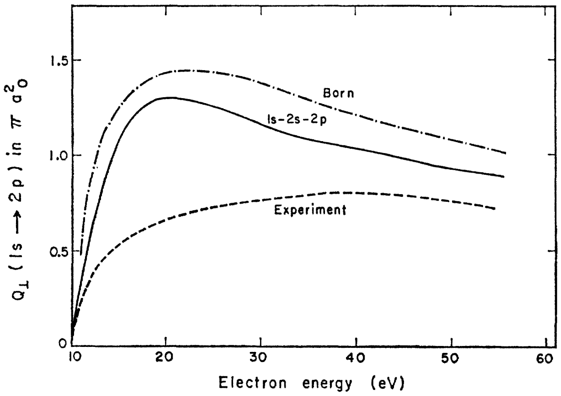

FIG. 1. Total $1s-2p$ excitation cross section as a function of incident electron energy as given by the Born approximation and by the present calculation. Experimental results are those of Fite and Brackmann, and of Fite, Stebbings, and Brackmann.

The disagreement between our calculation and the experimental results led us to investigate the $1s-2p$ excitation cross section with various combinations of closely coupled atomic-hydrogen states other than $1s-2s-2p$ (see Sec. V). We find, however, that other combinations never yield results different from the $1s-2s-2p$ values by more than about 10%. Since we are in a position of having to explain away discrepancies of more than a factor of two, we feel that no close-coupling approximation such as the present one will yield results for the $1s-2p$ excitation cross section which agree satisfactorily with measured values.

Our results for the polarization of the emitted photons and the experimental measurements of this quantity as given by Fite and Brackmann[12] are presented in Fig. 2. Theory predicts a rather large drop in polarization at 11.0 eV just above threshold. For energies slightly lower than these the curve must rise again—and steeply—to fulfill the requirement of the theory that $P=3/7$ at threshold. Thus, it appears that near threshold the polarization must be a rapidly varying and nonmonotomic function of energy. It must be admitted that this conclusion is based, in part, upon the 11.0-eV point which, because of our difficulty in achieving convergence, is perhaps less reliably given than points at other energies. Nonetheless, there is no question that we do see a distinct flattening of the polarization curve for energies somewhat higher than

---

[16] W. L. Fite, R. F. Stebbings, and R. T. Brackmann, Phys. Rev. **116**, 356 (1959).

11.0 eV where no convergence problem casts doubt upon the calculated results.

From Fig. 2 it is plain that agreement between theory and measurement for the polarization of the emitted photons is poor. In view of the large errors quoted in the experimental results, we cannot regard this disagreement as strong evidence against the validity of the close-coupling approximation.

In our investigation of the $1s-2p$ excitation cross section we discovered that results obtained by use of a closely coupled wave function containing only the $1s$ and $2p$ states agree very well with those obtained by using our standard $1s-2s-2p$ expansion (Table V). This agreement emboldens us to calculate the $1s-3p$ excitation cross section by using a close-coupling expansion that includes only the $1s$ and $3p$ states. The results, presented in row (b) of Table V and shown in Fig. 3, though probably not the last word in accuracy, should not be egregiously erroneous. There are no experimental data for comparison, but once again, as in the case of the $1s-2p$ cross section, there is fairly good (though accidental?) agreement above 30 eV between our close-coupling result and the Born approximation values given by Lichten and Schultz[14] which are shown in Fig. 3.

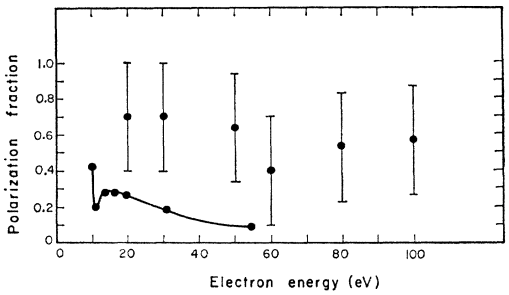

FIG. 2. Polarization of radiation emitted in $1s-2p$ excitations as a function of incident electron energy. Experimental points are those of Fite and Brackmann.

The large $1s-3p$ peak value at 15 or 16 eV, if it is to be believed, has interesting consequences for the $1s-2s$ excitation cross section, for it would mean that electron bombardment excites the hydrogen atom into the $3p$ state more readily than had been anticipated in earlier estimates. This, in turn, will result in an enhanced $2s$ population coming from $3p-2s$ radiative transitions. Although we postpone to Sec. IIIC a detailed discussion of this point, we may remark here that this effect brings close-coupling predictions of the $1s-2s$ cross section into greater disagreement with experiment than had been suspected.

None of the results presented in this subsection are in satisfactory agreement with experiment. Yet we find that the higher angular-momentum states make large contributions to the cross sections in question, and we have considerable confidence in our results for these states. Thus, we are at a loss to explain, for example, the serious discrepancy in the $1s-2p$ case, and feel that further experimental effort is well justified.

TABLE V. A comparison of the $1s-2p$ cross section in units of πa_0^2 at two energies using two methods of calculation: (a) the $1s-2p$ close-coupling approximation and (b) the $1s-2s-2p$ close-coupling approximation. The "Sum" column includes contributions from higher L values (not shown). All numbers include the appropriate spin-weighting factors.

k^2(au)	Spin \ L		0	1	2	3	4	Sum
1.0	Singlet	a	0.017	0.065	0.301	0.020	0.007	0.414
		b	0.036	0.110	0.253	0.035	0.010	0.448
1.0	Triplet	a	0.002	0.107	0.002	0.163	0.041	0.329
		b	0.000	0.080	0.046	0.167	0.044	0.351
2.25	Singlet	a	0.006	0.004	0.082	0.100	0.072	0.393
		b	0.017	0.018	0.094	0.100	0.070	0.428
2.25	Triplet	a	0.006	0.003	0.013	0.086	0.124	0.594
		b	0.011	0.013	0.036	0.108	0.134	0.664

C. The $1s-2s$ Excitation Cross Section

We turn our attention now to another excitation process of theoretical and experimental interest, that of the excitation of the $2s$ state of hydrogen from the ground state by electron impact. In Table VI, row (a), we give the results for the $1s-2s$ excitation cross section calculated in a $1s-2s$ close-coupling approximation by Marriott[17] for $L=0$, and by Smith[18] for higher L. In row (b) of Table VI we list our own results for the same quantity calculated in the $1s-2s-2p$ close-coupling approximation. We see that the effect of including the $2p$ state is to modify the $L>0$ partial-wave contributions to the cross section, and this modification for any L diminishes as the projectile energy increases away from the threshold. This behavior conforms to our expectations, since the $2p$ state accounts for an appreciable part of the long-range distortion

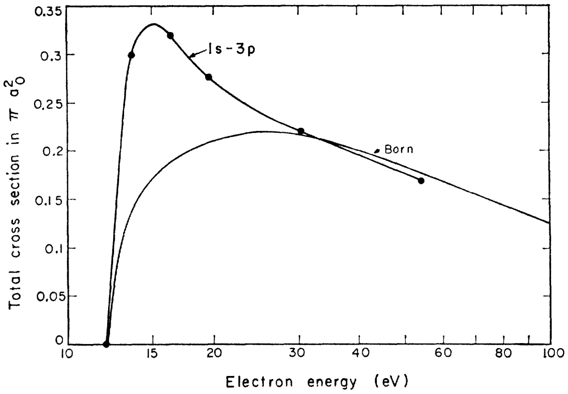

FIG. 3. Total $1s-3p$ excitation cross section as a function of incident electron energy as given by the present calculation and by the Born approximation (Lichten and Schultz).

---

[17] R. Marriott, Proc. Phys. Soc. (London) **72**, 121 (1958).

[18] K. Smith, Phys. Rev. **120**, 845 (1960).

TABLE VI. Partial-wave contributions to total $1s-2s$ excitation cross section in units of πa_0^2 calculated in (a) the $1s-2s$ close-coupling approximation and (b) the $1s-2s-2p$ close-coupling approximation; and the spin-flip cross section calculated in the $1s-2s-2p$ close-coupling approximation. The "Sum" column includes all significant partial-wave contributions. All numbers include spin-weighting factors.

k^2 (au)	Spin \ L		0	1	2	3	4	5	6	7	8	9	10	Sum	Spin flip
0.81	Singlet	a	0.038	0.008											≈0.157
		b	0.0529	0.0045	0.0581	≈0.003	0.0001							≈0.118	
	Triplet	a	0	0.1736	0.006										
		b	0.0012	0.0709	0.0031	0.0175	0.0030							0.0929	
1.00	Singlet	a	0.0714	0.051											0.2212
		b	0.0766	0.0145	0.0823	0.0103	0.0018	0.0003	0.0001					0.1858	
	Triplet	a	0.0027	0.161	0.046	0.002									
		b	0.0036	0.1219	0.0211	0.0208	00071	0.0012	0.0002					0.1758	
1.21	Singlet	a	0.070	0.0524	0.0003										0.1854
		b	0.0588	0.0246	0.0645	0.0232	0.0054	0.0014	0.0004	0.0001				0.1785	
	Triplet	a	0.0044	0.105	0.0262										
		b	0.0051	0.1000	0.0316	0.0069	0.0113	0.0042	0.0013	0.0004	0.0001			0.1610	
1.44	Singlet	a	0.0547	0.053	0.0053										0.1146
		b	0.0380	0.0256	0.0245	0.0247	0.0082	0.0028	0.0010	(0.0004)	(0.0002)	(0.0001)		0.1255	
	Triplet	a	0.0061	0.0735	0.0577										
		b	0.0055	0.0716	0.0358	0.0036	0.0103	0.0065	0.0029	(0.0011)	(0.0005)	(0.0002)	(0.0001)	0.1380	
2.25	Singlet	a	0.0238	0.0383	0.011										0 .0285
		b	0.0123	0.0309	0.0015	0.0040	0.0051	0.0037	0.0022	(0.0011)	(0.0007)	(0.0004)	(0.0002)	0.0624	
	Triplet	a	0.0073	0.0358	0.040										
		b	0.0045	0.0335	0.0302	0.0070	0.0045	0.0054	0.0046	(0.0033)	(0.0021)	(0.0012)	(0.0007)	0.0980	
4.00	Singlet	a	0.0073	0.0157											0.0059
		b	0.0049	0.0153	0.0068	0.0021	0.0010	0.0010	0.0010	0.0009	(0.0007)	(0.0005)	(0.0004)	0.0358	
	Triplet	a	0.0046	0.0162		0.0143									
		b	0.0030	0.0154	0.0175	0.0100	0.0045	0.0025	0.0021	0.0020	(0.0020)	(0.0016)	(0.0013)	0.0654	

which is known to have its greatest influence near thresholds and which, in addition, quite naturally manifests itself in states of larger L. That the $2p$ state also plays a role in allowing for short-range correlation effects is evidenced by its somewhat greater effect in the singlet-spin state (where short-range correlation is important) than in the triplet-spin state.

Table VI includes a "Sum" column for the total cross section and a column for the spin-flip cross section, the latter being given by Eq. (14). These sums include all significant partial waves, and for the higher energies in the $1s-2s-2p$ approximation, contributions up to L values of about 15 must be taken into account. Such large values of L are not required in the $1s-2s$ approximation where, due to neglect of the long-range effects represented by the $2p$ state, one is dealing with an effective interaction of short range. Thus, there is a significant difference between the contributions from high angular momenta in the two approximations. Despite these differences, however, the total $1s-2s$ excitation cross section is not much altered by the inclusion of the $2p$ state (see Fig. 1). The $1s-2s$ approximation does, indeed, yield a less pronounced peak than that given in the present calculation, but it occurs at about the same energy (≈14 eV) in both cases, and at no energy is the difference between the two calculations greater than a few percent.

Our results, as shown in Fig. 4, become almost indistinguishable from those given by the ordinary Born approximation at our highest energy (54.4 eV). However, the second Born approximation of Kingston, Moiseiwitsch, and Skinner, an approximation to the $1s-2s-2p$ method, which is an attempt to allow for virtual transitions between the first two hydrogen levels,[19] shows appreciable departures from our result at this energy. Apparently it is not possible to allow adequately for virtual transitions within the framework of a perturbation calculation; one must include strongly coupled states exactly.

There are two sets of experimental data shown in Fig. 4 with which we may compare our calculation. The first data, measurements made by Lichten and Schultz,[14] are not too different in magnitude from our own, although at lower energies there is a discrepancy of 20 to 25%. The second set of data is provided by Stebbings *et al.*[20] They disagree completely with our own insofar as magnitude is concerned, the discrepancy being as great as a factor of two-and-a-half at some energies. The shape of their curve, however, is not unlike our own.

The experimental data shown in Fig. 4 were subject to normalization. Those of the Stebbings group were normalized to Born approximation values between 200 and 700 eV, a procedure which, in principle, is to be preferred to that of Lichten and Schultz who normalized their data to Born values at 45 eV, an energy at which the validity of the Born approximation might seem questionable. Our calculation, however, agrees very well with the Born approximation for energies as low as 30 eV, and thus seems to justify the Lichten-Schultz normalization procedure.

There is one further point to be made with regard to the measured values of the $1s-2s$ excitation cross section. The methods used by Lichten and Schultz and by Stebbings require that raw experimental data be corrected for the enhancement of the $2s$ state population caused by radiative transitions from higher levels excited by the electron bombardment. The results shown in Fig. 4 have been subject to such a correction by use of an expression given by Lichten and Schultz

---

[19] A. E. Kingston, B. L. Moiseiwitsch, and B. G. Skinner, Proc. Roy. Soc. (London) **A258**, 254 (1960).

[20] R. F. Stebbings, W. L. Fite, D. G. Hummer, and R. T. Brackmann, Phys. Rev. **119**, 1939 (1960).

which takes into account only the effect of transitions from all higher lying p levels. They estimate that

$$\sigma_p(2s)=\sigma_T(2s)+0.21\sigma(3p),$$

where $\sigma_T(2s)$ is the calculated $1s-2s$ excitation cross section and $\sigma_p(2s)$ is the total cross section for excitation of the metastable $2s$ state by all processes. The quantity denoted $\sigma(3p)$ is the cross section for excitation of the $3p$ level; Lichten and Schultz obtain a value for this quantity by normalizing the Born approximation value by the ratio of $Q(1s\rightarrow 2p)$ given by Fite *et al.* to the Born approximation value of the same quantity. In the previous section we indicated that the experimental values of $Q(1s\rightarrow 2p)$ may be too small; corrected values would thus lead to values of $\sigma_p(2s)$ for which the theoretical-experimental discrepancy would be even worse than that shown in Fig. 4.

Another piece of experimental information available is the total spin-flip cross section. Lichten and Schultz find a ratio for spin-flip to total cross section of 0.9±0.1 at threshold. Our value is about 0.7, in fair agreement with measurement. A ratio such as this, incidentally, is not beset with normalization difficulties, and the relatively good agreement obtained here we regard as evidence in favor of our $1s-2s$ excitation results.

Our remarks should indicate that the situation with regard to the $1s-2s$ excitation cross section is far from satisfactory. We do not have as much confidence in our $1s-2s$ results as we do for our $1s-2p$, since, in the latter, higher angular-momentum contributions are more important and more accurately calculated. Despite this, we find it difficult to understand the large discrepancies discussed above within the framework of this kind of close-coupling approximation. We feel this situation warrants continued experimental effort. In particular, close scrutiny of normalization procedures involved in processing experimental data may prove fruitful.

D. Differential Cross Sections and Electron-Spin Polarizations and Correlations

In this section we present results for the $1s-1s$ and $1s-2s$ differential cross sections. We also give the functions of scattering angle defined in Sec. II in connection with the spin polarization and correlation. All quantities are calculated in the $1s-2s-2p$ close-coupling approximation. Apart from total cross sections, these quantities are, perhaps, the most easily measured of the various quantities which characterize electron-hydrogen collisions.

The results for the $1s-2s$ scattering are of more than ordinary interest because of the quite pronounced disagreement between experiment[14] and the present calculation. If this disagreement is the fault of the calculation, it must be ascribed mainly to the unusually large contributions we obtain from higher angular-momentum states. It is the sum of these large contributions that leads to predictions very much in excess of the measured values. Higher partial-wave contributions affect any angle-dependent quantity such as $\sigma(\theta)$ or $d(\theta)$ much more than they do a total cross section; thus, the functions given in this section are one obvious place to begin the search for the cause or causes of the discrepancy.

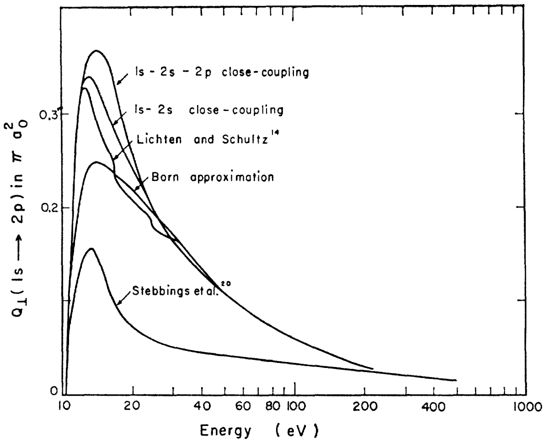

FIG. 4. Total $1s-2s$ excitation cross section as a function of incident electron energy as given by various calculations and by two sets of experiments.

However, if the disagreement is ascribed to some flaw in the experiments, such as difficulty in normalizing the data properly, then the experimental measurement of, for example, the $1s-2s$ differential cross section will still play a vital role in revealing the source of the disagreement; the angular distribution, normalized correctly or not, provides much information about the contributions of higher partial waves. Even more informative in this respect is the depolarization ratio which, by its definition [Eq. (14)], is independent of normalization.

In Fig. 5 we plot the angular distribution for the elastic scattering of electrons by atomic hydrogen in its ground state for incident electron energies of 13.6, 19.6, and 30.6 eV. At the higher energies the scattering is largely confined to the forward cone. The depolarization ratio for the same reaction is given in Fig. 6. The large backward dip at the lower energies tends to disappear as the energy increases and $d(\theta)$ tends to unity for all angles. This limiting high-energy behavior follows as a consequence of the equality of the singlet and triplet amplitudes at high energies, a manifestation of the waning influence of exchange as the energy increases. In Figs. 7–10 we give the functions $m(\theta)$, $n(\theta)$, $p(\theta)$, and $q(\theta)$ which are defined in Eq. (11).

In Fig. 11 we plot the differential $1s-2s$ excitation cross section. Again, as in the corresponding elastic case, the distribution is almost all in the forward direction at higher energies. However, unlike the elastic case, there is an appreciable backward peak at the lower energies. A significant feature of these distributions is

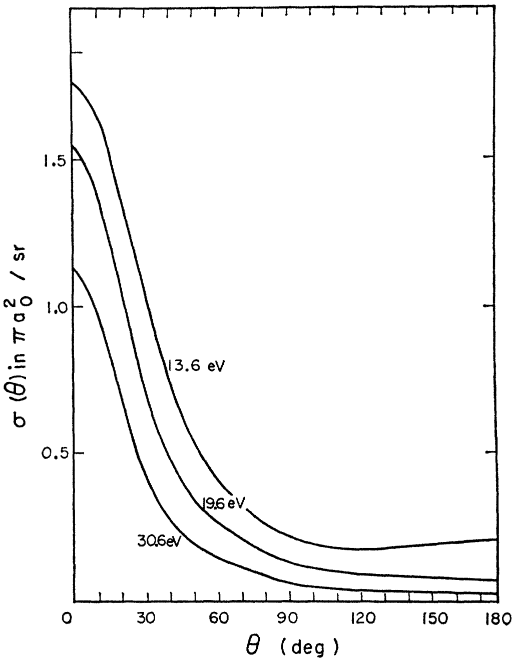

FIG. 5. Differential cross section for elastic $1s-1s$ scattering as a function of scattering angle for three incident electron energies. Note that this cross section is identical with the function $k(\theta)$ defined in Eq. (11).

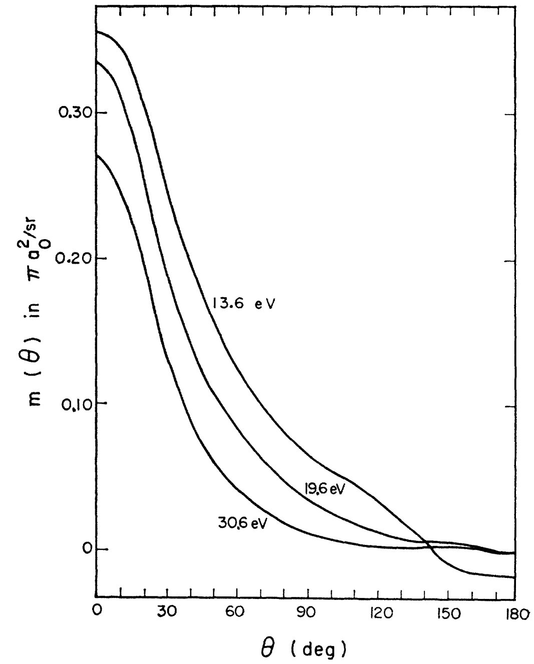

FIG. 7. The quantity $m(\theta)$ for elastic $1s-1s$ scattering as a function of scattering angle for three incident electron energies.

the nonisotropy at energies only slightly above the $1s-2s$ excitation threshold. Even at these low energies the higher ($L>0$) partial-wave contributions dominate the behavior of the cross section, and an angular distribution might, therefore, help resolve the $1s-2s$ discrepancy between calculation and experiment.

Finally, in Fig. 12 we give the $1s-2s$ depolarization ratio. An important feature of this ratio at all energies

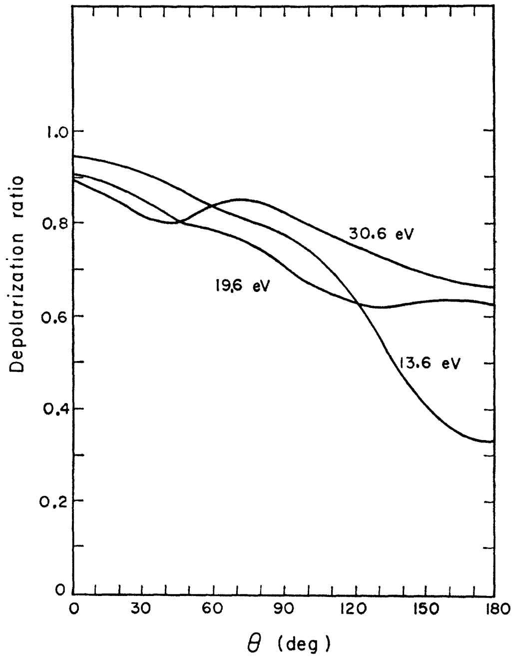

FIG. 6. The depolarization ratio for elastic $1s-1s$ scattering as a function of scattering angle for three incident electron energies.

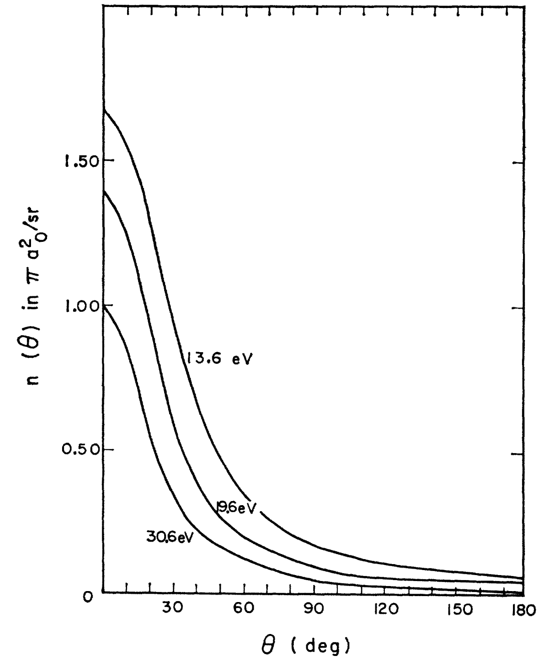

FIG. 8. The quantity $n(\theta)$ for elastic $1s-1s$ scattering as a function of scattering angle for three incident electron energies.

considered is the large dip in the angular range from 30 to 60 deg. This dip becomes less pronounced (although it remains quite appreciable) and moves to smaller angles as the energy increases.

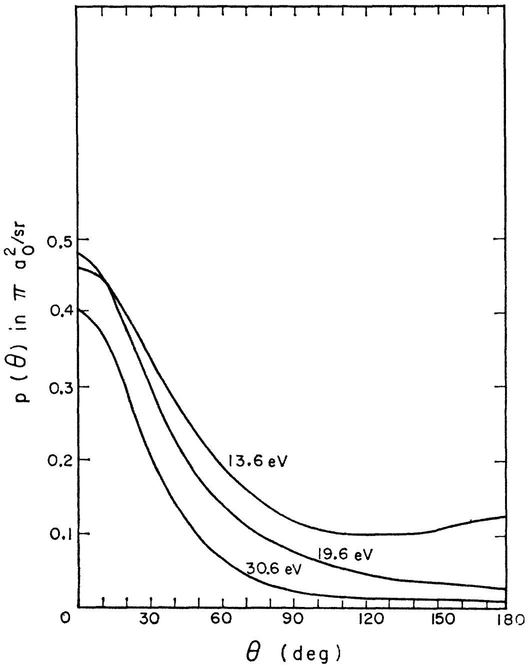

FIG. 9. The quantity $p(\theta)$ for elastic $1s-1s$ scattering as a function of scattering angle for three incident electron energies.

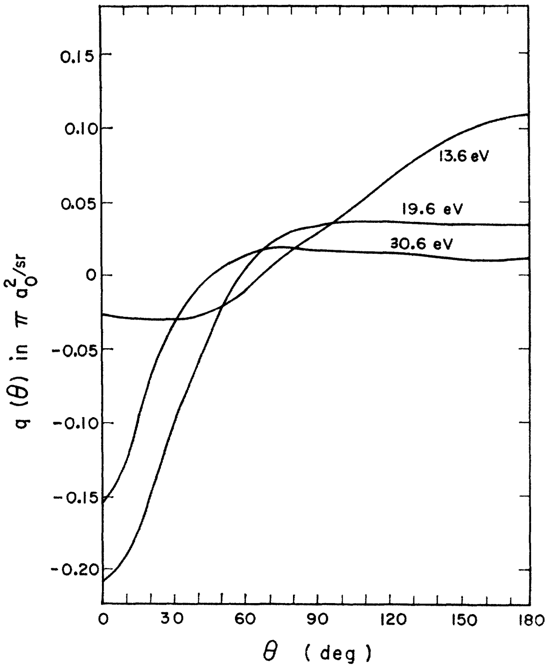

FIG. 10. The quantity $q(\theta)$ for elastic $1s-1s$ scattering as a function of scattering angle for three incident electron energies.

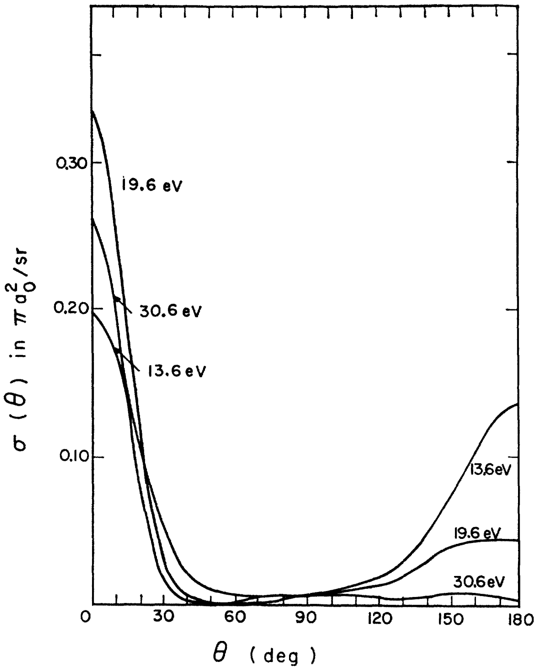

FIG. 11. Differential $1s-2s$ excitation cross section as a function of scattering angle for three incident electron energies. Note that this cross section is identical with the function $k(\theta)$ defined in Eq. (11).

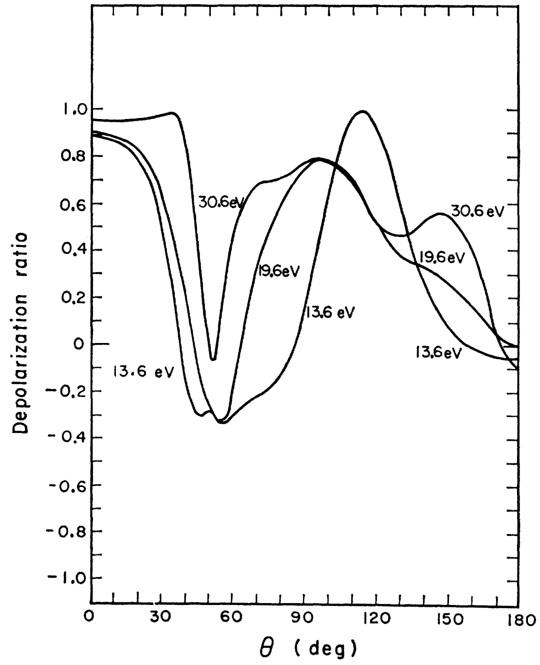

FIG. 12. The depolarization ratio for $1s-2s$ excitation as a function of scattering angle for three incident electron energies.

IV. ELASTIC AND INELASTIC SCATTERING OF POSITRONS BY ATOMIC HYDROGEN

We now consider the elastic and inelastic scattering of positrons by atomic hydrogen for incident positron

TABLE VII. Total elastic and inelastic cross sections for the scattering of positrons by atomic hydrogen in units of πa_0^2. Values in rows "a" calculated in the $1s-2s$ close-coupling approximation, those in row "b" in the $1s-2s-2p$ close-coupling approximation. Figures in parentheses indicated number of partial waves taken into account.

k^2 (au)		$Q(1s\rightarrow 1s)$			$Q(1s\rightarrow 2s)$			$Q(1s\rightarrow 2p)$		
0.81	a	0.679(0)		0.750(5)	0.003(0)		0.004(5)			
	b	0.585(0)		0.628(6)	0.007(0)		0.059(6)	0.005(0)		0.072(6)
1.00	a	0.608(0)	0.689(4)		0.009(0)	0.019(4)				
	b	0.541(0)	0.582(4)	0.594(9)	0.007(0)	0.131(4)	0.146(9)	0.011(0)	0.201(4)	0.266(9)
1.21	a	0.542(0)		0.632(7)	0.015(0)		0.035(7)			
	b	0.496(0)	0.543(4)	0.557(12)	0.009(0)	0.159(4)	0.195(12)	0.013(0)	0.304(4)	0.496(12)
1.44	a	0.487(0)	0.586(5)		0.019(0)	0.049(5)				
	b	0.453(0)	0.514(5)	0.522(13)	0.012(0)	0.193(5)	0.218(13)	0.012(0)	0.494(5)	0.694(13)
2.25	a	0.356(0)	0.475(6)		0.021(0)	0.072(6)				
	b	0.343(0)	0.431(6)	0.436(16)	0.017(0)	0.182(6)	0.208(16)	0.005(0)	0.620(6)	0.995(16)
4.00	a	0.220(0)	0.349(7)		0.012(0)	0.067(7)				
	b	0.218(0)	0.332(7)	0.334(17)	0.012(0)	0.119(7)	0.138(17)	0.001(0)	0.448(7)	0.920(17)

energies between 11 and 54.4 eV. Other above-threshold calculations have been made by Moiseiwitsch and Williams[8] who treat the elastic scattering of fast ($E>217.6$ eV) positrons using a simplification of the second Born approximation, and by Smith *et al.*,[9] who consider both elastic and inelastic collisions in the $1s-2s$ close-coupling approximation. Our calculation is also carried out in a close-coupling approximation, one that includes $1s$, $2s$, and $2p$ states of hydrogen; positronium formation is neglected.

Calculations of positron-hydrogen cross sections are of considerable interest despite the fact that, as yet, no experimental data are available for purposes of comparison. This interest stems in part from the contrast between electron-hydrogen scattering and positron-hydrogen scattering. In particular, the mean static interaction (the total potential averaged over the hydrogen ground state) and the long-range "polarization potential" have opposite signs for positrons but have the same sign for electrons. An investigation by Cody *et al.*[21] shows that the positron-hydrogen scattering length is negative which, in accordance with the standard convention, implies that the effective positron-hydrogen interaction at zero energy is positive (see also Rosenberg and Spruch).[22]

Another important feature of positron-hydrogen collisions is that, while there are no effects analogous to electron exchange, the possibility of positronium formation arises; with it arises the question of the relative importance of (a) positronium formation and (b) the distortion represented by the $2p$ state in modifying the effect of the static interaction. We should like, of course, to take into account both effects, at least in some approximation, but we have chosen to treat the $2p$-state distortion effects and omit consideration of positronium formation. We make this choice because the apparatus necessary for such a calculation becomes available by quite simple modifications of the code that was developed and used to treat electron-hydrogen collisions. The inclusion of positronium formation, on the other hand, would require revisions of our methods. While our choice is thus dictated by convenience, it can be justified on physical grounds: First, 68% of the long-range distortion is accounted for by including the $2p$ hydrogen state in the close-coupling expansion. Second, according to the low-energy ($E<6.8$ eV) positron-hydrogen analyses of Cody and Smith,[21] the inclusion of the $2p$ state has a greater influence on the scattering than does virtual positronium formation for processes in which there is a hydrogen atom in the initial and final states. For these reasons we feel that the present calculation, based on a $1s-2s-2p$ close-coupling approximation, will yield physically significant results even though it fails to account for positronium formation.

In Table VII we present the cross sections for the scattering of positrons by atomic hydrogen calculated in both the $1s-2s$ and the $1s-2s-2p$ close-coupling approximations. We see that, as the energy of the incident positron decreases and approaches the first inelastic threshold from above, the two approximations differ more and more. Thus, at 54.4 eV for elastic scattering the two approximations agree within 1%, but at 11.00 eV the agreement is not even within 10%. A deviation of the same order is also observed in the $1s-2s$ excitation cross section, but here, even at 54.4 eV, there are large discrepancies between the two approximations for a few of the lower partial waves. These discrepancies are more pronounced in individual partial-wave cross sections than in total cross sections where they tend to cancel. The same kind of discrepancies (though not so large) as well as the same tendency to cancel in total cross sections are also to be found in electron-hydrogen collisions.

For the calculation of the optically allowed $1s-2p$ transition we found it necessary at the highest energy to take into account partial-wave contributions up to and including $L=17$ to obtain convergence. This is at least twice as many as are required in most other parts of the calculation and strongly suggests that in this

---

[21] W. J. Cody and K. Smith, Argonne National Laboratory Report ANL-6121, 1960 (unpublished); see also W. J. Cody, Argonne National Laboratory Report ANL/AMD-21, 1961 (unpublished).

[22] L. Rosenberg and L. Spruch, Phys. Rev. 120, 474 (1960).

TABLE VIII. The $L=0$ singlet cross section in units of πa_0^2 evaluated at two energies in various close-coupling approximations: (a) $1s$; (b) $1s-2s$; (c) $1s-2p$; (d) $1s-3p$; (e) $1s-2s-2p$; (f) $1s-2s-2p-3s$; (g) $1s-2s-2p-3p$; (h) $1s-2s-2p-3d$; (i) $1s-2s-2p-3s-3p$. All numbers include the spin-weighting factors.

k^2 (au)	Process	a	b	c	d	e	f	g	h	i
1.0	$1s-1s$	0.2666	0.286	0.2962	0.2661	0.2635	0.2910	0.2731	0.2640	0.3001
	$1s-2s$	...	0.0714	...	...	0.0766	0.0687	0.0598	0.0633	0.0486
	$1s-2p$	...	...	0.0166	...	0.0360	0.0196	0.0316	0.0497	0.0255
1.44	$1s-1s$	0.1633	0.140		0.1596	0.1269	0.1281	0.1303	0.1274	0.1314
	$1s-2s$	...	0.0547	...	...	0.0380	0.0273	0.0414	0.0389	0.0300
	$1s-2p$	...	...		...	0.0343	0.0421	0.0254	0.0313	0.0335

range of energy partial-wave analysis alone ceases to be useful and should be replaced by, perhaps, the Born approximation supplemented with close-coupling results for lower angular momenta.

V. CONVERGENCE IN CLOSELY COUPLED STATES

Because of the discrepancies between experiment and theory, we have investigated the effects on the $L=0$ contributions to the cross section which are introduced by hydrogen states other than the $1s$, $2s$, and $2p$. Attention is limited to the $L=0$ state chiefly in the interest of simplicity—each new hydrogen state introduced couples in only one unknown scattering-wave function. However, we hope our results will provide some general indications of the accuracy of the close-coupling approximation. Since our code, in its present form, can cope with a maximum of five coupled equations (mainly because of computer-space limitations) we have also confined our attention to combinations of states from only the first three hydrogen levels.

Our results are presented in Table VIII where we give our calculated values for the $L=0$ contributions to the $1s-1s$, $1s-2s$, $1s-2p$ cross sections. We have used nine different close-coupling combinations, as indicated in the table, and have considered two energies above the second-quantum excitation level.

The elastic $1s-1s$ cross section is only slightly modified from its $1s-2s-2p$ value by the inclusion of states from the third quantum level, although the values given by the $1s-2s$ and $1s-2p$ approximations are appreciably different. The agreement is better at the higher energy.

The cross sections for the $1s-2s$ and $1s-2p$ excitations are also only slightly changed by the inclusion of additional states, once both the $2s$ and $2p$ states are present in the close-coupling wave function; however, these cross sections are not given as accurately as are those in the elastic case.

These brief considerations, though they may be only another case of the slow convergence in hydrogen eigenstates already noted by Burke and Schey[2] for energies below the first excitation threshold, do give us some hope that the $1s-2s-2p$ close-coupling approximation can provide reasonable results. Evidently we can gain little in calculating $1s-2s$ and $1s-2p$ excitation cross sections by including hydrogen eigenstates coming from the third, or higher, levels. However, in the interest of accuracy, it does appear important to include all hydrogen states corresponding to any given level. Thus, one should include the $2p$ state in calculating $Q(1s\rightarrow 2s)$, and the $2s$ state in calculating $Q(1s\rightarrow 2p)$.

We emphasize that these remarks rest on an investigation which involves only the state $L=0$. It would be interesting to see if they apply to other states as well.

VI. CONCLUSIONS

We have calculated quantities pertaining to the collisions of electrons and positrons with atomic hydrogen for incident projectile energies from 11.0 to 54.4 eV. Calculations were made mainly by means of the $1s-2s-2p$ close-coupling approximation.

There are no experimental data in the case of elastic scattering of electrons. There are data, however, for the inelastic processes $1s-2s$ and $1s-2p$; agreement is poor in both cases. For purposes of calculating the $1s-2p$ excitation cross section, our approximation is, we believe, quite accurate. Consequently, we suggest further experimental effort. For $1s-2s$ excitations, our method is inherently less accurate, although we have presented evidence which indicates that more extensive close-coupling methods, including, for example, $3s$, $3p$, and $3d$ states, would yield results essentially no better than those we have obtained in our $1s-2s-2p$ approximation. We are left, then, with the conclusion that either the method of calculation must be radically altered or replaced with something quite different, or the experiments must be repeated with close attention paid to normalization procedures. The fact that our method gives the ratio of spin flip to total cross section (a quantity independent of normalization) in fair accord with experiment, and since our prediction of the shape, if not the magnitude, of the $1s-2s$ cross sections accords well with measurement, we are led, not unnaturally, to prefer the latter alternative.

For positrons we have no experimental results for comparison. We have pointed out, however, certain differences with the corresponding positron case. The $2p$ state, for instance, seems to play a more important role in the $1s-2s$ excitation process here than it does for electrons.

Our results can be compared with those coming from the Born approximation as given by Seaton *et al.* In terms of R-matrix elements, good agreement is obtained for $L \geqslant 6$ at all energies considered. However, for lower angular-momentum states almost no similarity exists between our numbers and those coming from the Born approximation. It is surprising, therefore, to find such close agreement in the two calculations, in the case of electrons, for total $1s-2s$ and $1s-2p$ excitation cross sections. Seaton's calculation is a first Born approximation sometimes modified to preserve unitarity. Because a second Born approximation made by Kingston, Moiseiwitsch, and Skinner[19] does not improve matters, we conclude that perturbation methods may not be of great value in dealing with strongly coupled states.

The elastic $1s-1s$ cross section results for electrons and positrons are not greatly modified by the inclusion of the $2s$ and $2p$ states, although we believe our results, including these states, are probably accurate within a few percent.

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. Sidney Fernbach and Dr. William Miller for making available to us extensive computing facilities for this work. We also acknowledge the programming assistance afforded us by D. F. Jordan and S. Zawadzki and most particularly by Samuel F. Mendicino whose patient, painstaking, and always accurate work over a long period has been instrumental to the successful completion of this undertaking. We are pleased to acknowledge our correspondence with Dr. M. J. Seaton who pointed out the existence of work in progress similar to our own. Finally, one of us (PGB), extends to Dr. David Judd and the members of the Theoretical Physics Group at Berkeley his thanks for the hospitality extended him during his sojourn in the United States.

APPENDIX

We give in Table IX (p. 1273) R-matrix elements for electron-hydrogen scattering obtained in our $1s-2s-2p$ close-coupling approximation. Our notation conforms to that of Seaton *et al.*[15] For a given total angular momentum L there are five states designated by the index ν and given as follows:

ν	nl_1	k	l_2	L
1	$1s$	k_1	l	l
2	$2s$	k_2	l	l
3	$2p$	k_2	$l-1$	l
4	$2p$	k_2	$l+1$	l
5	$2p$	k_2	l	l

The quantity denoted k_1 is the wave number in the incident channel, and $k_2^2 = k_1^2 - 0.75$. The state denoted $\nu = 5$ is not coupled to any other and is of interest only for a determination of $2p-2p$ transition rates. Since we have not considered such transitions, we have not calculated the associated matrix element R_{55}. For $L \neq 0$, states $\nu = 1, 2, 3, 4$ are coupled and give rise to a symmetric 4×4 R matrix. When $L=0$, however, the state $\nu = 3$ is not involved and the dimensionality of the R matrix is then 3×3; in this case the missing elements are recorded as zeros in Table IX.

Table IX lists results for both singlet and triplet scattering. At $k^2 = 0.81$, 1.0, and 1.21, we give values for $L=0$ to 5; at $k^2 = 1.44$ and 2.25 for $L=0$ to 6; and at $k^2 = 4$ for $L=0$ to 7. In only one case, $L=3$ singlet at $k^2 = 0.81$, did our iteration method fail to converge; the entries for this case are results interpolated from neighboring k^2 and L values and are probably accurate to about 10%. The $k^2 = 0.81$ values were, at all L and in both spin states, the most difficult to obtain, and the results at this energy in those cases in which convergence was achieved are expected to be accurate to about 2 or 3%. At all other energies we believe the accuracy to be better than 1%.

To evaluate the $1s-2p$ and the $2s-2s$ excitation cross sections given in the body of the paper, contributions from angular momenta higher than those given in the table are required. For this purpose we use Born-approximation results calculated by Seaton *et al.*[15] (which are fairly accurate for $L \geqslant 6$ or 7) supplemented by $1s-2s-2p$ close-coupling no-exchange results (which are readily obtained with our code) for L values up to about 15 at the highest energy.

TABLE IX. Reactance matrix elements calculated in the $1s-2s-2p$ close-coupling approximation for six electron energies above threshold. See Appendix for description of notation.

	R_{11}	R_{12}	R_{13}	R_{14}	R_{22}	R_{23}	R_{24}	R_{33}	R_{34}	R_{44}
$k^2=0.81$ Singlet										
$L=0$	0.8189	−0.2763	0	0.5863	−1.0994	0	1.0211	0	0	0.5841
1	−0.0560	−0.0070	0.1596	−0.0591	0.6131	0.0020	0.5759	−0.8728	−0.6716	−1.0264
2	−1.2834	−1.8061	10.695	−3.7558	−2.1310	15.004	−5.6676	−82.956	29.565	−11.605
3	≈0.03	≈ 0	≈−0.00	≈0.004	≈0.01	≈0.75	≈−0.7	≈0.6	≈0.15	≈−0.75
4	+0.0107	0.0001	−0.0064	0.0005	0.0317	0.4733	−0.4566	0.4399	0.0169	−0.3641
5	0.0057	0.0001	−0.0014	−0.0004	0.0146	0.3885	−0.3769	0.2718	0.0162	−0.2427
$k^2=0.81$ Triplet										
$L=0$	16.655	−0.3650	0	0.3940	−0.6858	0	−0.0094	0	0	1.4022
1	0.4098	0.1860	0.0699	0.3315	−0.3167	−0.5277	−1.1184	0.6800	−2.2293	−3.1550
2	0.0686	−0.0415	−0.0098	−0.0243	0.6684	1.2533	−0.4545	0.1447	0.5451	−1.1398
3	0.0287	0.0114	−0.0742	0.0148	0.1314	0.4895	−0.5315	1.2602	−0.1056	−0.5763
4	0.0109	0.0005	−0.0080	0.0008	0.0345	0.4674	−0.4551	0.4558	0.0136	−0.3633
5	0.0057	−0.0002	−0.0015	0	0.0147	0.3881	−0.3768	0.2727	0.0161	−0.2426
$k^2=1.0$ Singlet										
$L=0$	0.2891	−0.0059	0.0000	+1.7014	0.0184	0.0000	+1.4779	0.0000	0.000	−5.5243
1	−0.0160	−0.1564	−0.1742	−0.5403	0.3901	0.9745	1.1385	1.2562	2.2451	0.5796
2	0.1447	0.0671	−0.3623	0.2294	0.5420	0.4618	−0.3424	1.3645	−0.5159	−1.1545
3	0.0360	−0.0012	−0.1031	0.0186	0.0185	0.6801	−0.6861	0.4310	0.1738	−0.8646
4	0.0149	0.0002	−0.0410	0.0051	0.0387	0.4670	−0.4780	0.3166	0.0636	−0.4432
5	0.0076	0.0001	−0.0174	0.0016	0.0242	0.3763	−0.3858	0.2198	0.0402	−0.2838
$k^2=1.0$ Triplet										
$L=0$	7.2054	4.5532	0.0000	−2.5610	16.781	0.0000	−10.317	0.0000	0.0000	6.2190
1	0.5704	−0.7812	−0.3791	−0.5817	4.8984	2.0335	3.1094	0.3618	0.8896	2.2052
2	0.0695	−0.1040	0.2716	−0.0977	0.8925	1.2522	0.0208	−6.8871	1.3483	−0.5346
3	0.0370	0.0180	−0.1441	0.0334	0.4537	0.1954	−0.2622	1.2761	−0.2678	−0.4271
4	+0.0152	0.0047	−0.0488	0.0080	0.1321	0.3643	−0.4066	0.4684	−0.0083	−0.3854
5	0.0077	0.0011	−0.0193	0.0021	0.0444	0.3530	−0.3726	0.2533	0.0263	−0.2747
$k^2=1.21$ Singlet										
$L=0$	0.1443	0.5051	0.0000	+1.6317	0.1545	0.0000	−0.5242	0.0000	0.0000	−5.9143
1	−0.0352	−0.2222	0.0016	−0.4943	0.5497	0.9197	0.8650	−0.3344	1.4811	−0.1953
2	0.1385	0.0372	−0.4403	0.2197	0.6649	0.4610	−0.0424	1.0982	−0.3949	−0.7879
3	0.0416	0.0151	−0.1683	0.0505	0.1315	0.5670	−0.6064	0.4121	0.1493	−0.9043
4	0.0188	0.0034	−0.0778	0.0141	0.0669	0.4368	−0.4703	0.2765	0.0776	−0.4855
5	0.0099	0.0009	−0.0403	0.0051	0.0344	0.3638	−0.3877	0.1920	0.0541	−0.3122
$k^2=1.21$ Triplet										
$L=0$	3.8892	0.5389	0.0000	−0.1942	1.0557	0.0000	−1.4925	0.0000	0.0000	0.7018
1	0.5011	−0.4922	−0.2499	−0.2857	3.3613	1.3002	1.3528	−0.5887	0.3358	0.9143
2	0.1099	−0.0643	−0.3593	−0.0004	0.9102	−0.0685	0.1476	6.3689	−0.7887	−0.0141
3	0.0401	−0.0020	−0.1527	0.0243	0.4960	0.2089	−0.1711	1.0480	−0.2087	−0.2931
4	0.0188	0.0047	−0.0850	0.0140	0.2203	0.2922	−0.3251	0.4746	−0.0405	−0.3321
5	0.0100	0.0023	−0.0424	0.0058	0.0899	0.3100	−0.3428	0.2603	0.0160	−0.2724
$k^2=1.44$ Singlet										
$L=0$	0.2624	0.7389	0.0000	+0.8292	−0.4261	0.0000	−1.5288	0.0000	0.0000	−2.9887
1	−0.0160	−0.3206	0.0538	−0.4079	0.8996	1.0677	0.6438	−1.1786	1.2674	−0.1574
2	0.1125	0.0189	−0.4712	0.1707	0.7111	0.3541	0.0809	1.1423	−0.3691	−0.4009
3	0.0403	0.0178	−0.2037	0.0666	0.2889	0.4265	−0.4079	0.4626	0.0436	−0.6927
4	0.0208	0.0065	−0.1071	0.0239	0.1276	0.3835	−0.4156	0.2769	0.0588	−0.4610
5	0.0118	0.0024	−0.0623	0.0101	0.0598	0.3399	−0.3713	0.1838	0.0541	−0.3187
6	0.0071	0.0009	−0.0381	0.0047	0.0300	0.3014	−0.3241	0.1296	0.0456	−0.2296
$k^2=1.44$ Triplet										
$L=0$	2.8588	0.4270	0.0000	−0.0879	0.0746	0.0000	−1.3268	0.0000	0.0000	0.3798
1	0.4640	−0.3508	−0.1997	−0.1884	2.5955	1.0886	0.8208	−1.2793	0.3090	0.6843
2	0.1117	−0.0859	−0.2087	−0.0175	0.8577	0.1362	0.0769	3.0325	−0.3669	0.0351
3	0.0422	−0.0160	−0.1541	+0.0185	0.5008	0.2081	−0.1336	0.9202	−0.1676	−0.1901
4	0.0208	0.0010	−0.1002	0.0169	0.2700	0.2528	−0.2622	0.4653	−0.0552	−0.2635
5	0.0118	0.0025	−0.0626	0.0097	0.1326	0.2738	−0.3039	0.2669	0.0024	−0.2474
6	0.0071	0.0015	−0.0390	0.0050	0.0630	0.2708	−0.2969	0.1661	0.0238	−0.2044

TABLE IX (*continued*)

	R_{11}	R_{12}	R_{13}	R_{14}	R_{22}	R_{23}	R_{24}	R_{33}	R_{34}	R_{44}
$k^2=2.25$ Singlet										
$L=0$	0.1199	1.4076	0.0000	+0.7505	−3.7442	0.0000	−3.0550	0.0000	0.0000	−1.5274
1	0.0453	−0.4175	0.3105	−0.2410	1.0097	2.0162	−0.0245	−6.9787	2.0573	−0.1582
2	0.0474	−0.0482	−0.3461	0.0710	0.7669	0.1290	0.0955	1.2149	−0.2899	0.0648
3	0.0275	−0.0092	−0.2124	0.0564	0.4641	0.2186	−0.1191	0.5535	−0.0963	−0.1667
4	0.0186	0.0013	−0.1456	0.0374	0.2788	0.2438	−0.2232	0.3231	−0.0212	−0.2295
5	0.0128	0.0028	−0.1040	0.0236	0.1633	0.2498	−0.2626	0.2057	0.0143	−0.2260
6	0.0090	0.0022	−0.0761	0.0148	0.0943	0.2449	−0.2669	0.1374	0.0295	−0.1989
$k^2=2.25$ Triplet										
$L=0$	1.6284	0.5991	0.0000	+0.1035	−2.4569	0.0000	−1.9941	0.0000	0.0000	−0.1209
1	0.4118	−0.1984	−0.1577	−0.0870	1.5766	1.4653	0.2185	−5.9655	0.8500	0.4535
2	0.1264	−0.0950	−0.1377	−0.0140	0.8137	0.1184	0.0445	1.6006	−0.2211	0.1977
3	0.0479	−0.0396	−0.1402	0.0133	0.5109	0.1637	−0.0774	0.7476	−0.1245	0.0074
4	0.0232	−0.0135	−0.1197	0.0196	0.3349	0.1856	−0.1564	0.4402	−0.0672	−0.0938
5	0.0137	−0.0031	−0.0954	0.0172	0.2144	0.2019	−0.2051	0.2784	−0.0254	−0.1387
6	0.0091	0.0003	−0.0738	0.0128	0.1327	0.2105	−0.2273	0.1823	0.0016	−0.1485
$k^2=4.00$ Triplet										
$L=0$	0.8383	−1.1673	0.0000	−0.5836	5.5326	0.0000	+1.9726	0.0000	0.0000	1.4729
1	0.1417	−0.2220	−0.1507	−0.0332	1.2489	−0.4376	0.2813	4.3772	−0.7055	0.5643
2	0.0478	−0.0960	−0.1735	0.0237	0.7166	0.0493	0.0541	1.0251	−0.1920	0.2546
3	0.0218	−0.0451	−0.1547	0.0354	0.4963	0.1051	−0.0321	0.5716	−0.1120	0.1057
4	0.0137	−0.0206	−0.1335	0.0352	0.3574	0.1325	−0.0907	0.3694	−0.0662	0.0135
5	0.0094	−0.0087	−0.1136	0.0306	0.2574	0.1498	−0.1317	0.2515	−0.0341	−0.0434
6	0.0070	−0.0031	−0.0962	0.0251	0.1838	0.1605	−0.1582	0.1757	−0.0113	−0.0748
7	0.0055	−0.0007	−0.0814	0.0200	0.1296	0.1661	−0.1728	0.1246	0.0041	−0.0892
$k^2=4.00$ Triplet										
$L=0$	1.2202	−0.9043	0.0000	−0.4699	7.2115	0.0000	+2.4055	0.0000	0.0000	1.7000
1	0.3621	−0.1469	−0.0344	−0.0546	1.3364	−0.4214	0.2262	4.7021	−0.5486	0.5790
2	0.1397	−0.0891	−0.0929	−0.0071	0.7381	0.0605	0.0331	1.1013	−0.1580	0.3011
3	0.0580	−0.0542	−0.1064	0.0119	0.5084	0.0991	−0.0334	0.6340	−0.1051	0.1569
4	0.0275	−0.0306	−0.1064	0.0198	0.3709	0.1183	−0.0791	0.4200	−0.0720	0.0631
5	0.0145	−0.0160	−0.0991	0.0215	0.2735	0.1326	−0.1138	0.2912	−0.0455	0.0005
6	0.0088	−0.0077	−0.0886	+0.0201	0.2007	0.1435	−0.1390	0.2063	−0.0242	−0.0391
7	0.0061	−0.0033	−0.0776	0.0173	0.1455	0.1509	−0.1553	0.1477	−0.0079	−0.0620