Scattering of electrons by hydrogen atoms

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The cross sections for elastic scattering and for excitation of hydrogen atoms by electron impact are calculated for energies in the range from 10.2 to 12.1 eV. The calculations are made variationally. A pseudostate expansion is employed to represent the target atom. Energies and widths of resonances are obtained. Results are compared with experiment.

I. INTRODUCTION

This paper is devoted to a study of the scattering of electrons by hydrogen atoms in an energy range in which the states with principal quantum number n=2 can be excited, but no other inelastic processes occur. A significant comparison of theory and experiment ought to be possible in this energy region between the n=2 and 3 thresholds, free of complications, both experimental and theoretical, which may arise at higher energies when cascade processes and ionization are possible.

The paper reports an attempt to perform a rather precise calculation which covers the specific range of incident energies from $k^2 = 0.7501$ (0.0001 Ry above the n=2 threshold), through $k^2=0.8885$ (0.000 39 Ry below the n=3 threshold). Emphasis is placed on determination of the total cross sections for the excitation of the 2s and 2p state since rather accurate experimental data are available.¹⁻² We also give the total cross section for elastic scattering. There is a shape resonance just above the n=2 threshold, and there are series of Feshback resonances under the n=3 threshold. The positions and widths of 24 resonances in partial waves from ${}^{1}S$ through ${}^{3}F$ have been determined. Some of the ones which are found in the ${}^{1}P$ state are the same as those observed in measurements of the photodetachment of the H^- ion.³

The present calculation employs variational procedures.⁴ It is based on a close-coupling expansion including pseudostates. Over almost all of the energy range a basis of 7s, 5p, 3d, 2f, and 1g states have been used to describe the atom. This 18-state basis includes the exact hydrogenic eigenfunctions through n=3 plus the exact atomic 4f state and, in addition, includes 11 pseudostates (4s, 3p, 2d, 1f, and 1g types). The parameters of this basis are given in Table 7 of Ref. 4.

There have been many previous scattering calculations in this range. The present work is, in fact, an extension of a calculation by Morgan *et al.*, 5which used a very similar approach, but a smaller (14-state) basis set. That work considered only the region of the Feshbach resonances under the n=3threshold. We have extended their calculation through the entire region between the n=2 and 3 thresholds. In addition, it has been possible to include more short-range functions in expansion of the scattering wave function used in the variational method here than in the previous work. As a result, better convergence and more accurate results have been obtained. Some of the Feshbach resonances have been located more accurately, and some others found for the first time in scattering calculations. The increased accuracy of the present calculations has also made it possible to describe the shape resonance just above the n=2 threshold.

Other calculations deserve mention at this point. Geltman and Burke⁶ were the first to use a pseudostate basis for the description of the target in this energy range. They employed a small basis set containing six states: the exact 1s, 2s, and 2patomic states and three pseudostates denoted $\overline{3s}$. $\overline{3p}$, and $\overline{3d}$. These pseudostates were those derived previously by Damburg and Geltman⁷ and provide the full polarizabilities of most of the channels which open at the n=2 threshold. Geltman and Burke reported cross sections at only four energies. However, they compared their results at these energies with the six-state (exact atomic eigenfunction 1s through 3d) close-coupling calculation of Burke et al.,⁸ and with a calculation of Taylor and Burke⁹ in which the three eigenstate expansion (1s, 2s, 2p) was supplemented by variationally determined correlation terms of the Hylleras type. I

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will show subsequently a comparison of eigenphase sums from the present work and from the calculation discussed by Geltman and Burke, which suggests that the present results may indeed be more accurate than any of the preceding ones. It is worth noting at this point that our calculated cross sections are closer to those of Taylor and Burke than either of the six-state calculations mentioned above.

In Sec. II, I will discuss briefly some of the calculational procedures, and make the comparison with the previous calculations just mentioned. Section III contains a list of the resonances obtained in this work. Their positions and widths are compared with other theoretical results and with experiment where possible. Results for the scattering cross sections are presented and discussed in Sec. IV. My conclusions are given in Sec. V.

II. PROCEDURES, COMPARISON OF CALCULATIONS

The procedure of the variational methods as applied to hydrogen are discussed in some detail in Ref. 4. It is not necessary to repeat this material here. The following comments should serve to characterize this calculation adequately.

With one exception, discussed below, this work is based on the 18-state (7-5-3-2-1) target-state expansion. Parameters are contained in Table 7 of Ref. 4. Computations were made for values of the total angular momentum L from 0-3. Contributions from states with $L \ge 4$ were obtained from the unitarized Born approximation including exchange (UBX). A model polarization potential¹⁰ is included in the calculation of the 1s-1s element of the UBX K matrix. In the energy range studied here, the contribution from these higher angular momenta ought to be small, and the UBX extension should not lead to significant error. In the "worst" case, at the high-energy end of our range $(k^2=0.888)$ the $L \ge 4$ contribution to the 1s-2p excitation cross section is about 2%, and for the 1s-2s, about 0.5%. The major error produced by inadequate treatment of the higher partial waves is that we are unable to investigate the resonances which may occur in the ${}^{1}G$ state.

Efforts were made to improve the convergence of the expansion of the scattering wave functions with respect to the situation reported in Ref. 5. The improved convergences is manifest in improved agreement between cross sections computed according to the five variational procedures considered^{4,11} [Kohn, Inverse Kohn, orthogonalized minimum norm (OMN), inverse orthogonalized minimum (IOMN), optimized anomaly free (OAF)] (see Refs. 4 and 11 for a discussion of different variational procedures). The improvements resulted from the following measures: (1) The number of short-range function [Slater-type orbitals (STO)] used in the expansion of the scattering wave functions was increased from 9 for each channel, as used in Ref. 5 to 15 (for L=0 and 1), 13 for L=2, and 12 for L=3. (2) Additional energy-dependent oscillatory functions (proportional to $\frac{\sin kr}{r^3}$ and $\cos kr / r^3$ at large r) were included in the expansion basis for L=2 and 3 in addition to the functions varying as r^{-2} at large r used in previous work. (3) Portions of the calculation of the inverse of the "bound-bound" matrix⁴ were performed in quadruple precision (on an IBM 3033).

The exceptional case mentioned above occurred for the ¹P state in the region where a shape resonance occurs, just above the n=2 threshold. In this region a smaller, 11-state (5-4-2) basis was used for the target. (The parameters are also contained in Table 7 of Ref. 4.) This was done in order to permit use of a large basis (20 STO's) set in the expansion of the scattering wave function. Oscillatory functions decaying as r^{-3} and as r^{-2} were also included. The large basis was necessary in order to obtain adequate agreement between the different variational estimates of the K matrix.

Calculations were made on a grid of energies in which $\Delta E = 0.005$ Ry from $k^2 = 0.75$ to 0.855 for all angular momenta considered. Above this, a grid of $\Delta E = 0.001$ Ry was used from $k^2 = 0.8880$, and then intervals of 0.0001 Ry up to $k^2 = 0.8885$. Additional calculations were made in the vicinity of resonances. For example, the ${}^{1}P$ (and ${}^{3}P$) partial cross sections were calculated at intervals of 0.0001 Ry from $K^2 = 0.7501 - 0.7525$, then at more widely spaced points $(k^2 = 0.7530, 0.7535, 0.754, 0.755, 0.755, 0.754, 0.755$ 0.756, 0.757, and 0.758) up to $k^2 = 0.76$. Other partial cross-sections $(^{1,3}S, ^{1,3}D)$ which are large but not resonant in the near threshold region were calculated at intervals of about 0.001 Ry up to $k^2 = 0.76$. In the region just below the n = 3threshold, calculations were made in the vicinity of each of the Feshbach resonances on a grid whose size was determined roughly by the width of the resonance. As examples, the ${}^{3}F$ cross sections were calculated at nine closely spaced energies in the neighborhood of the spectacular resonance at $k^2 = 0.8770$, and the ¹D cross sections were obtained at 12 points close to the resonance at $k^2 = 0.88849.$

It remained to place the cross sections on a uniform scale suitable for tabulation, and graphical display. A K-matrix fitting routine, previously developed in another context¹² was used for interpolation in the neighborhood of a resonance. In this procedure, the K-matrix pole is first located by examination of the original calculations. Once this position is known, a linear least-squares fit is then made to the K matrix in which the background energy dependence is expressed as a low-order polynomial. Cross sections can then be computed rapidly from the fitted K matrix at any desired energy.

The quality of different calculations can, in part be compared through consideration of the eigenphase sum.⁶ It is known¹³ that the exact values of the tangents of the eigenphases are upper bounds on results which can be obtained from a closecoupling calculation in which exact target wavefunctions are used in all open channels. Here we shall consider the sum of the eigenphases. It can further be shown that the addition of a closed channel function to the target basis must lead to an increase in this quantity. Hence, there is a sense in which that calculation which produces the highest eigenphase sum is best. There is one proviso, however; the tangent of an eigenphase, which is the quantity actually computed by diagonalization of the K matrix, is a periodic function with singularities. The arctangent is multivalued. The comparison of eigenphase sums between two calculations is therefore meaningful only if the corresponding eigenphases in each refer to the same branch of the arctangent.

Eigenphase sums from different calculations are presented in Table I for L=0, 1; S=0, 1 at four energies below the resonance region. Three of the calculations are those discussed by Geltman and Burke and mentioned above. Results from our earlier work with the 11-state (5-4-2) basis¹⁴ are also given. In most instances the present eigenphase sums are larger than those previously reported. There is an apparent anomaly in the ³S state for $k^2=0.76$ where the result of Taylor and Burke appears to be much larger. This is, however, a situation in which one has to be careful about choosing

TABLE I. Eigenphase sums for four states at four energies. T.B.: Taylor and Burke; 3-state + correlation functions, Refs. 6 and 9; G.B.: Geltman and Burke; three exact states + three pseudostates, Ref. 6; 6cc: six atomic states, Refs. 6 and 8; 5-4-2: 11-state basis set previously employed in Ref. 14.

<i>k</i> ²	Present	G.B.	Т.В.	6 <i>cc</i>	5-4-2
			¹ S		
0.76	-0.462	-0.535	-0.508	-0.574	-0.47
0.78	1.701	1.620	1.640	1.576	1.68
0.81	1.649	1.559	1.618	1.518	1.62
0.83	1.656	1.562	1.615	1.498	1.62
			³ S		
0.76	1.030	1.024	2.634	1.012	1.01
0.78	2.953	2.947	2.924	2.936	2.94
0.81	2.112	2.104	2.097	2.084	2.10
0.83	1.721	1.714	1.693	1.692	1.71
			1 P		
0.76	-1.122	-1.152	-1.185	-1.245	-1.19
0.78	0.645	0.614	0.559	0.538	0.64
0.81	-0.327	-0.360	-0.417	-0.468	-0.36
0.83	-0.727	-0.760	-0.826	-0.869	-0.75
			³ P		
0.76	-0.417	-0.439	-0.508	-0.476	-0.44
0.78	1.482	1.455	1.386	1.410	1.46
0.81	0.682	0.651	0.683	0.584	0.66
0.83	0.436	0.398	0.312	0.320	0.40

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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Ε	Г		Ε	Г	Ε	Γ	Ε
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			S=0				L=0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.861 70	2.84(-3)		0.862 00ª	2.83(-3)	0.8621	2.86(-3)	0.861 99
$\begin{array}{cccccccccccccccccccccccccccccccccccc$).885 37				5.82(-4)	0.88461	6.11(-4)	0.88445
$\begin{array}{cccccccccccccccccccccccccccccccccccc$).887 63						1.55(-4)	0.88773
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$).88802						6.74(-5)	0.887 99
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			S=1				L = 0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.88204				1.8(-5)	0.882 12	1.77(-5)	0.88203
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.887 53				9(-6)	0.887 87	4.28(-6)	0.887 52
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			S=0				L = 1	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1.04(-3)		0.751 30 ^b			1.47(-3)	0.75121
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.875 32	2.34(-3)		0.874 58°	2.42(-3)	0.87495	2.39(-3)	0.874 57
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.882 86				9(-6)	0.88297	1.79(-5)	0.882 86
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.887 77				2.2(-5)	0.88815	4.36(-6)	0.887 77
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0.888 24				1.62(-4)	0.888 40	1.37(-4)	0.888 20
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			S=1				L=1	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.863 72	3.2(-3)		0.864 20 ^c	3.40(-3)	0.86428	3.29(-3)	0.864 16
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.885 05				6.38(-4)	0.88526	6.11(-4)	0.88516
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.887 25						8.39(-6)	0.887 24
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0.888 17						1.22(-4)	0.888 18
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			S=0				L = 2	
0.88636 $4.83(-4)$ 0.88647 $4.89(-4)$ 0.88849 $5.37(-5)$ 0.88869 $4.2(-5)$	0.868 33	3.2(-3)		0.8681 ^d	3.24(-4)	0.8682	3.27(-3)	0.868 09
$0.888 49 \qquad 5.37(-5) \qquad 0.888 69 \qquad 4.2(-5)$	0.88636				4.89(-4)	0.88647	4.83(-4)	0.88636
	0.888 52				4.2(-5)	0.888 69	5.37(-5)	0.88849
L=2 $S=1$			S=1				L=2	
$0.88207 \qquad 7.5(-4) \qquad 0.88212 \qquad 7.55(-4) \qquad 0.88204^{d} \qquad 7.5(-4)$	0.881 22	7.5(-4)		0.882 04 ^d	7.55(-4)	0.882 12	7.5(-4)	0.88207
0.88453 $1.70(-5)$ 0.88463 $1.7(-5)$	0.884 52				1.7(-5)	0.884 63	1.70(-5)	0.884 53
$0.888 21 \qquad 3.15(-6) \qquad 0.888 58 \qquad 6(-6)$	0.888 22				6(-6)	0.888 58	3.15(-6)	0.888 21
L=3 $S=0$			S=0				L=3	
0.886 89 1.0(-5) 0.887 01 1.0(-5)	0.886 88				1.0(-5)	0.88701	1.0(-5)	0.886 89
L = 3 $S = 1$			S=1				L=3	
0.87697 2.18(-4) 0.8772 2.3(-4) 0.87698 ^d 2.2(-4)	0.875 77	2.2(-4)		0.876 98 ^d	2.3(-4)	0.8772	2.18(-4)	0.87697
0.88800 $1.08(-5)$ 0.88806 $1:0(-5)$	0.88793				1.0(-5)	0.88806	1.08(-5)	0.888 00

TABLE II. Results of several different calculations for energies and widths of resonances (all quantities in Rydbergs). The number in parentheses indicates the power of 10 by which the preceding quantity is to be multiplied.

^aReference 18.

^bReference 22.

^cReference 19.

^dReference 20.

the correct branch of the arctangent function. Let us follow the rise of the eigenphase as the n=2threshold is approached from the high energy side. A more complete examination of the ³S eigenphase sum in our calculations shows that, as the incident energy decreases toward the n=2 threshold, the eigenphase sum rises. Just below $k^2=0.78$, one of the component eigenphases rises to $\pi/2$. Below this energy, the computer program selects a value for the eigenphase close to $-\pi/2$, and the rise with decreasing energy continues. Apparently the ³S eigenphase sum in the calculations of Taylor and Burke has not undergone this change and is on a different branch.

III. RESONANCES

Scattering calculations lead to very direct determinations of positions and widths of resonances. I examine the eigenphase sums for each L and S for evidence of a rapid increase. Calculations are then made in the region of the resonance, and a fit is made to the eigenphase sum δ_T using the expression

$$\delta_T(E) = a + \tan^{-1} \frac{\Gamma}{2(E_R - E)} . \tag{1}$$

The quantity E_R is the resonance energy and Γ is the width. I attempt to place the calculated points close enough to E_R so that the variation of the nonresonant background with energy is negligible.

This procedure works quite satisfactorily for the Feshbach resonances lying under the n=3 threshold. It is, however, unsatisfactory for the ¹P shape resonance just above the n=2 threshold, which I have discussed elsewhere.¹⁵ In this case the background eigenphase sum is falling rapidly with increasing energy, apparently as $1/(E - E_{\rm th})$ from a presumably infinite value at the threshold energy $E_{\rm th}=0.75$ Ry. In this case, I replace (1) with

$$\delta_T(E) = \frac{a}{E - E_{\rm th}} + b + c \left(E - E_{\rm th}\right) + \tan^{-1} \frac{\Gamma}{2(E_R - E)} .$$
(2)

The present results for the positions and widths of the calculated resonances are given in Table II, where they are compared with values from the previous scattering calculation of Morgan *et al.*⁵ Generally, the resonance energies determined here are slightly lower than those of Morgan *et al.*⁵ as one would expect, in view of the increase of the eigenphase sum as the target basis is improved. It would be outside of the intended scope of this paper to review all the extensive previous work on the determination of resonances (see Refs. 16 and 17 for reviews). I will, however, present results obtained by Ho using the complex rotation method, $^{18-20}$ for the lowest members of the Feshbach resonance series for the ^{1}S , ^{1}P , ^{3}P , ^{1}D , ^{3}D , and

 ${}^{3}F$ states. Generally, excellent agreement is seen in the comparison for both the positions and the widths. I also present results for the energies (only) of all the resonances found here from the compilation of Lipsky, Anania, and Conneely.²¹ These authors diagonalize the Hamiltonian for the two-electron system in a basis formed from angularly coupled products of hydrogenic functions, the ground state and the n=2 states being excluded. They do not obtain widths, and a shift of the resonance position resulting from interactions with open channels is also not included in their method. This shift is presumably similar in magnitude to the width. All of the resonances they find below $k^2 = 0.8885$ with the conventional parity $(-1)^L$ have been found in these scattering calculations. It will be seen that the difference between my energies and those of Ref. 21 is in magnitude typically less than the width and therefore for some of the higher, narrow resonances the agreement is really excellent.

The ¹P shape resonance above n=2 is, as usual, in a category by itself. I give in Table II, in addition to my result, the value obtained using the complex rotation method by Wendoloski and Reinhardt.²² In this case the agreement between the different techniques is not as good (particularly for the width) as was obtained for the Feshbach series. One may speculate whether the complex rotation method which employs a basis set of Laguerre functions with a common exponential factor may have some difficulty in describing a situation in which there is a strong energy-dependent background.

The energy I reported previously²³ for the position of the (very narrow) lowest ¹P Feshbach resonance below the n=2 threshold can be subtracted from that given here for the shape resonance to give a separation between these two resonances of 0.003 31 Ry or 0.0450 eV. This result seems to be in good agreement with preliminary results²⁴ from precise measurements of the photodetachment of H⁻.

Some of the resonances reported here have been observed in electron-scattering experiments. The discussion of scattering observations will be deferred to Sec. IV in which results for cross sections will be presented. It should be noted that the two broadest of the Feshbach resonances in ¹P state under the n=3 threshold have been observed in measurements of the H⁻ photodetachment cross section.³ The results of Hamm *et al.* for energies (after subtraction of the binding energy of H⁻) are

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k ²	1 <i>s</i> -1 <i>s</i>	1 <i>s</i> -2 <i>s</i>	1 <i>s</i> -2 <i>p</i>
0.7502	7.010	0.103	0.145
0.7504	7.016	0.106	0.165
0.7506	7.026	0.118	0.200
0.7508	7.040	0.137	0.256
0.7510	7.055	0.164	0.336
0.7512	7.064	0.194	0.423
0.7514	7.061	0.214	0.479
0.7516	7.047	0.217	0.489
0.7518	7.031	0.209	0.467
0.7520	7.017	0.198	0.435
0.753	6.981	0.159	0.323
0.754	6.964	0.146	0.278
0.755	6.954	0.140	0.256
0.756	6.945	0.137	0.244
0.758	6.910	0.135	0.230
0.76	6.909	0.136	0.224
0.765	6.859	0.138	0.218
0.77	6.815	0.141	0.219
0.775	6.770	0.145	0.224
0.78	6.727	0.149	0.231
0.785	6.683	0.155	0.238
0.79	6.639	0.162	0.246
0.795	6.595	0.169	0.254
0.80	6.552	0.176	0.261
0.805	6.509	0.184	0.269
0.81	6.467	0.190	0.279
0.815	6.422	0.195	0.288
0.82	6.318	0.200	0.298
0.825	6.340	0.204	0.309
0.83	6.298	0.207	0.320
0.835	6.257	0.210	0.330
0.84	6.216	0.212	0.341
0.845	6.176	0.213	0.349
0.85	6.136	0.212	0.361
0.855	6.101	0.205	0.367
0.858	6.092	0.191	0.365
0.860	6.120	0.166	0.354
0.861	6.171	0.145	0.345
0.862	6.210	0.148	0.348
0.863	6.156	0.174	0.356
0.864	6.139	0.188	0.358
0.865	6.109	0.220	0.376
0.866	6.055	0.233	0.374
0.867	6.014	0.215	0.332
0.868	6.000	0.179	0.268

TABLE III. Results for states 1s-1s, 1s-2s, and 1s-1p.

<i>k</i> ²	1 <i>s</i> -1 <i>s</i>	1 <i>s</i> -2 <i>s</i>	1 <i>s</i> -2 <i>p</i>
0.869	6.009	0.178	0.279
0.870	6.007	0.199	0.331
0.871	5.998	0.213	0.363
0.872	5.987	0.221	0.381
0.873	5.976	0.227	0.386
0.874	5.965	0.226	0.355
0.875	5.956	0.216	0.312
0.876	5.950	0.211	0.324
0.877	5.979	0.466	0.805
0.878	5.924	0.234	0.425
0.879	5.919	0.226	0.414
0.880	5.912	0.222	0.411
0.881	5.907	0.217	0.408
0.882	5.912	0.212	0.429
0.883	5.903	0.208	0.430
0.884	5.965	0.168	0.404
0.885	5.949	0.188	0.408

TABLE III. (Continued.)

 $E_R = 0.8748 \pm 0.0003$ Ry, $\Gamma = 0.00202 \pm 0.00006$ Ry for the lower of the two, and $E_R = 0.8886 \pm 0.0003$ Ry, $\Gamma = 0.00012 \pm 0.00002$ Ry for the higher.

IV. SCATTERING CROSS SECTIONS

Table III presents numerical values for the calculated elastic-scattering and excitation cross sec-



FIG. 1. Cross section (units πa_0^2) for the excitation of the 2s state in the energy range $0.75 \le k^2 \le 0.86$. Points represent the experimental results of Williams (Ref. 2).

tions at selected energies from $k^2 = 0.7502$ to 0.885. Above the latter energy, the structure in the excitation cross sections occurs on such a fine energy scale that an adequate tabulation would have to be very lengthy, and results are presented in graphical form instead. However, a more detailed tabulation can be obtained from the author on request.

First, a few brief comments about the elastic-



FIG. 2. Cross section (units πa_0^2) for the excitation of the 2p state in the energy range $0.75 \le k^2 \le 0.86$. Points represent the experimental results of Williams (Ref. 2).



FIG. 3. Same as Fig. 1 for the energy range $0.855 \le k^2 \le 0.8875$. Vertical bars indicate the position of resonances.



FIG. 4. Same as Fig. 2 for the energy range $0.855 \le k^2 \le 0.8875$. Vertical bars indicate the position of resonances.



FIG. 5. Same as Fig. 1 for the energy range $0.8875 \le k^2 \le 0.8885$. (Calculated cross sections only.)

scattering cross section. Inspection of Table III shows that resonances produce only small oscillations in this quantity, superimposed on a steadily decreasing background. Elastic scattering in this energy range is dominated by contributions from the two states ${}^{3}S$, and ${}^{3}P$ which together account for (very roughly) about 85% of the total. Slightly less than 10% of the total comes from ${}^{1}S$, and all the other partial waves contribute together roughly 5%. Neither of the dominant states has major resonant structure in the elastic channel. The elastic cross section is so smooth and so nearly monotonic that I have not shown it graphically.

On the other hand, the excitation cross sections have rich structure. It is useful to divide the total energy range into three separate regions in which different energy scales are appropriate for graphical purposes.

A. From threshold to the Feshbach resonance region

Figures 1 and 2 show the 2s and 2p excitation cross sections from $k^2 = 0.75$ to 0.86. The theoretical values are compared with the measurements of Williams.² The principal structure is that of the highly asymmetric, near threshold ¹P shape resonance. This resonance is clearly present in the experimental data which, however, show the smearing effects of a finite spread of electron energies. Above the shape resonance, the cross sections rise steadily until the Feshbach resonances begin. The calculations agree quite well with experiment in this range.



FIG. 6. Same as Fig. 2 for the energy range $0.8875 \le k^2 \le 0.8885$. (Calculated cross sections only.)

B. Lower resonance region

Figures 3 and 4 show the excitation cross sections from $k^2 = 0.855$ to 0.8875 Ry. The lower energy portions of the cross sections are dominated by a few broad resonances, (¹S, ³P, ¹D, and ¹P) and a high but rather narrow ³F resonance. The lower resonances are obviously present in the experimental data, although the calculated structure is clearly somewhat smeared in the experiments. The ³F resonance, which is a spectacular feature of the calculated cross sections is not apparent in the experimental results. As an energy increases, the calculated resonances become narrower and more closely spaced. The experimental results fail to reveal the predicted detailed structure.

C. Upper resonance region

Figures 5 and 6 show the excitation cross sections on a finer scale from $k^2 = 0.8875$ to 0.8885, the upper limit of the present calculations. Experimental results are very sparse and are not shown. The most pronounced structure is the second ${}^{3}F$ resonance whose width is only 10^{-5} Ry. This produces a factor of 2 enhancement of both the 2s and 2p cross sections. The depression as the highenergy end is approached is due to a ${}^{1}D$ resonance.

V. CONCLUSIONS

The present calculations are clearly able to account for the observed 2s and 2p total excitation cross section in the energy range between the n=2 threshold and the onset of the Feshbach resonances below the n=3 threshold. This application of variational methods to a close-coupling calculation with a reasonably large pseudostate basis is successful. Furthermore, the method appears to be quite effective in determining the positions and widths of resonances insofar as one can judge by the comparison of results calculated according to quite different methods. There is reasonable agreement with the corresponding quantities determined

from measurements of the photodetachment of H^- . It remains to be seen, however, whether the complicated and detailed structure predicted for the excitation cross sections in the region of the Feshbach resonances can be observed in electron-scattering experiments, for which still better energy resolution is required. Beyond this, measurements of the elastic-scattering cross section and of differential cross section in this energy range would be useful as additional tests of the adequacy of these calculations, and of current theory.

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