J. Phys. B: Atom. Molec. Phys., Vol. 8, No. 13, 1975. Printed in Great Britain.

Scattering of electrons by hydrogen atoms at intermediate energies: total and differential cross sections for excitation of $n = 2$ states

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Received 1 April 1975

Abstract. The results of a pseudostate expansion for low-order partial waves ($0 \leqslant L \leqslant 3$) are combined with the distorted-wave polarized-orbital method for higher partial waves in order to obtain cross sections for excitation of the 2s and 2p levels of atomic hydrogen by electron impact for incident energies in the range 10–30 eV. Both total and differential cross sections are calculated. Results are also presented for Lyα polarization and for the total cross section for all scattering processes.

1. Introduction

This paper is the fourth of a series of reports concerning the calculation of the scattering of electrons in the 10–30 eV range by atomic hydrogen using a variational method applied to a pseudostate expansion. The procedures of this work are described in detail in the first paper of this series (Callaway and Wooten 1974) which emphasizes application to elastic scattering. The results of this work for states of total angular momentum $0 \leqslant L \leqslant 3$ were subsequently combined with the Born exchange approximation for higher angular momenta to give the total cross section for 1s–2s and 1s–2p excitation from 10 to 20 eV (Callaway and Wooten 1975). The elastic differential cross section has been studied both experimentally and theoretically in the 10–30 eV range by Callaway and Williams (1975). The present work is concerned with total and differential cross sections for the excitation of the 2s and 2p states by electron impact in the range 10–30 eV. The total cross section for all scattering processes has also been estimated for energies in this range.

The variational pseudostate calculation as presently programmed becomes quite time consuming as the total angular momentum L increases. For this reason, this calculation has been limited to $L \leqslant 3$. This is sufficient to give a good determination of the total elastic cross section and a reasonable estimate of the 1s–2s total excitation cross section, but it is insufficient to determine the 1s–2p total cross section above about 13 eV, and it is insufficient to determine differential cross sections anywhere in the range considered. In this paper, the distorted-wave polarized-orbital method (DWPO) (McDowell *et al* 1974, 1975) has been used to determine the contribution from higher values of the total angular

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momentum. The combination gives results for the total and differential cross sections for excitation of the 2s and 2p states, and for the total cross section for all scattering processes.

2. Theoretical and numerical procedures

The pseudostate calculation and the DWPO method have been fully described in the references cited above. We will limit our discussion here to a brief survey of the essential features, and to the procedures used in combining the two approaches.

The pseudostate calculation represents the hydrogen atom by a set of eleven states, including the exact 1s, 2s, 2p and 3d atomic states plus seven pseudostates: three of s-type, three of p-type, and one of d-type. These states are a set of orthogonal approximate eigenfunctions found by diagonalizing a matrix representing the Hamiltonian for the isolated atom on a basis of Slater-type orbitals. The parameters of the basis functions and the energies of the pseudostates are given by Callaway and Wooten (1974).

Expansion in this set of states leads to a problem involving nineteen coupled channels if $L > 0$. The pseudochannels (as well as the real ones) are allowed to be open. In a calculation involving a smaller number of pseudostates, Burke and Webb (1970) demonstrated that such an approach leads to great improvement in the agreement between calculated and experimental excitation cross sections in comparison with the results of the three-state close-coupling approximation (Burke *et al* 1968); however, the use of open pseudostates may produce unphysical structure in the cross sections near the thresholds of open pseudochannels (Burke and Mitchell 1973). This problem is avoided by varying the parameters of the pseudostate set so as to move artificial thresholds away from the energies at which calculations are desired.

The coupled integro-differential equations of the pseudostate method are not solved directly in this work. Instead, variational estimates of the R matrix are made according to methods described by Nesbet (1969) and Nesbet and Oberoi (1972). For each of the energies and angular momenta considered here, variational calculations were made employing at least four and sometimes five methods: Kohn, inverse Kohn, OMN (optimized minimum-norm), IOMN (inverse OMN), and OAF (optimized anomaly-free). These methods are described in the references cited above. Results which showed obvious anomalies were discarded; the rest were averaged. All of the methods are stationary: that is, the error in the R matrix is of second order compared to the errors in the wavefunctions, but none give bounds in the energy range of interest here. The spread of the results gives some indication of the error in the variational calculation, or more properly, of the departure of the variational results from those which would be obtained by direct numerical integration of the coupled equations. This error depends on energy, angular momentum and spin of the states for which calculations are made, and appears to increase substantially as the number of open channels increases. In effect, the results show a tendency towards random scatter. The uncertainty in the elastic cross section is rather small, as it is dominated by states where the results are quite stable; however, the smaller excitation cross sections have an appreciable uncertainty, which is of the order of 5–10% for energies above 12 eV and about 2% from 10 to 12 eV.

The DWPO method as employed here produces singlet (+) and triplet (−) transition matrix elements

$$T_{if}^{\pm} = \langle \psi_f | V_f | (1 \pm P_{12}) \phi_i(1) F^{\pm}(2) + \phi_{pol}(1,2) F^{\pm}(2) \rangle \tag{1}$$

in which ψ_f is a wavefunction describing the final state in the absence of interactions, ϕ_i is the initial atomic function, ϕ_{pol} is the 'polarized orbital', dipole distortion only included, $F^{\pm}(2)$ is the scattering wavefunction obtained in the adiabatic exchange approximation, and V_f is the final-state interaction. Exchange polarization has been neglected. A detailed analysis of (1) has been given by McDowell *et al* (1974, 1975).

In the present work, we depart from previous practice by transforming the partial-wave expansion of $T_{if}^{\pm}$ from an uncoupled $(l_1 l_2 s_1 s_2)$ to a coupled $(l_1 l_2 L, S)$ representation. Let $F_{if}^{(S)}(L, l_{of}, l, l_{oi}, l')$ be the matrix element of the scattering amplitude in the coupled representation for a transition $i \to f$ in which the atomic electron has initial orbital angular momentum l_{oi}, and finally l_{of} and in which the free electron orbital angular momentum changes from l to l'. Let $T_{if}^{\pm}(l_{of} l, l_{oi}, l')$ be the corresponding matrix element of the T matrix in the uncoupled representation. Then for an s–p transition

$$F_{if}^{(S)}(L, 1, l; 0, l') = \frac{(-1)^{l+1}}{\sqrt{3}}(2l+1)^{1/2}\begin{pmatrix} l & l' & 1 \\ 0 & 0 & 0 \end{pmatrix}(k_f k_i)^{1/2} T_{if}^{\pm}(1, l; 0, l'). \quad (2)$$

Complex transition amplitudes were obtained from the pseudostate calculation for $0 \leqslant L \leqslant 3$, and combined with the results of the DWPO approach for $L \geqslant 4$. The results are described in the following sections.

3. Total cross sections

Partial cross sections according to the pseudostate approach for 1s–2s and 1s–2p excitation have been published elsewhere for $0{\cdot}75 \leqslant k^2 \leqslant 1{\cdot}44$. In table 1 we give the partial cross sections for $k^2 = 1{\cdot}69$, 1·96 and 2·25. Table 2 presents the contributions from the pseudostate and the DWPO calculations and their sum for $0{\cdot}85 \leqslant k^2 \leqslant 2{\cdot}25$. For $0{\cdot}76 \leqslant k^2 \leqslant 0{\cdot}83$ the higher partial-wave contributions have been obtained from Geltman and Burke (1970) and Burke *et al* (1967) as the DWPO approximation is unreliable in the resonance region. The results are shown graphically in figures 1 and 2. Experimental results are also presented. For the 2s excitation, the observations shown are those of Kauppila *et al* (1970) and Kochsmeider *et al* (1973). Oed (1971) has presented

Table 1. Partial cross sections (units of πa_0^2) for 1s–2s and 1s–2p excitation from the variational pseudostate calculation. Spin weighting factors are included.

	1s–2s							
k^2	$L=0$ $S=0$	$L=0$ $S=1$	$L=1$ $S=0$	$L=1$ $S=1$	$L=2$ $S=0$	$L=2$ $S=1$	$L=3$ $S=0$	$L=3$ $S=1$
1·69	0·0053	0·0033	0·013	0·018	0·000	0·016	0·006	0·001
1·96	0·0075	0·0030	0·017	0·018	0·000	0·019	0·004	0·0025
2·25	0·008	0·0028	0·010	0·015	0·002	0·018	0·003	0·004
	1s–2p							
1·69	0·016	0·0092	0·023	0·011	0·058	0·031	0·043	0·095
1·96	0·011	0·0092	0·020	0·011	0·047	0·028	0·046	0·076
2·25	0·008	0·0096	0·014	0·009	0·043	0·028	0·049	0·080

Table 2. Pseudostate and DWPO contributions to the cross sections for 1s–2s and 1s–2p excitation.

	1s → 2s			1s → 2p		
k^2	$\Sigma_0^3 \sigma(L)$ pseudostate	$\Sigma_4^\infty \sigma(L)$ DWPO	Total	$\Sigma_0^3 \sigma(L)$ pseudostate	$\Sigma_4^\infty \sigma(L)$ DWPO	Total
0·76	0·140	—	0·140	0·223[a]	(0·001)	0·224
0·78	0·151	—	0·151	0·219[a]	(0·012)	0·231
0·81	0·193	—	0·193	0·249[a]	(0·041)	0·290
0·83	0·214	—	0·214	0·277[a]	(0·054)	0·331
0·85	0·216	—	0·216	0·366	0·003	0·369
0·90	0·166	—	0·166	0·356	0·011	0·367
0·95	0·171	—	0·171	0·376	0·023	0·399
1·00	0·176	—	0·176	0·444	0·040	0·484
1·10	0·133	0·001	0·139	0·380	0·085	0·465
1·21	0·132	0·002	0·134	0·411	0·145	0·556
1·44	0·080	0·004	0·084	0·347	0·277	0·624
1·69	0·063	0·008	0·071	0·286	0·404	0·690
1·96	0·071	0·011	0·082	0·248	0·510	0·758
2·25	0·063	0·014	0·077	0·241	0·591	0·832

[a] Variational calculation through $L = 2$ only, contributions for $L \geqslant 3$ obtained from Geltman and Burke (1970), and Burke *et al* (1967). The variational contributions carry uncertainties as discussed in the text.

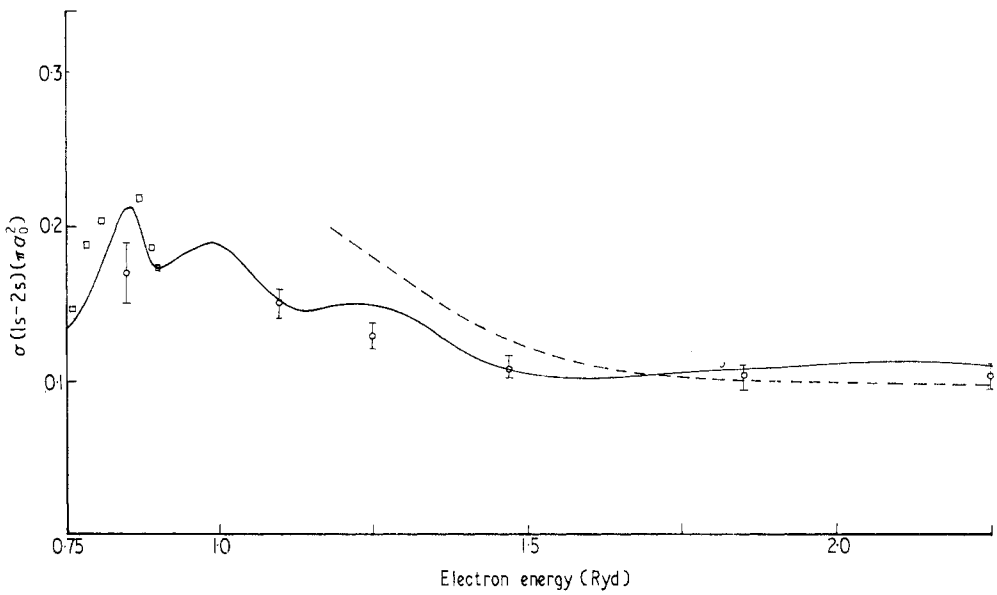

Figure 1. Total cross section (in units of πa_0^2) for

$$e + H(1s) \rightarrow e + H(2s).$$

The full curve represents the present result, the broken curve the calculation of Burke and Webb (1970). Both curves and the experimental measurements (⏀ Kauppilla *et al* 1970, □ Kochsmeider *et al* 1973) include an allowance for cascade, where relevant.

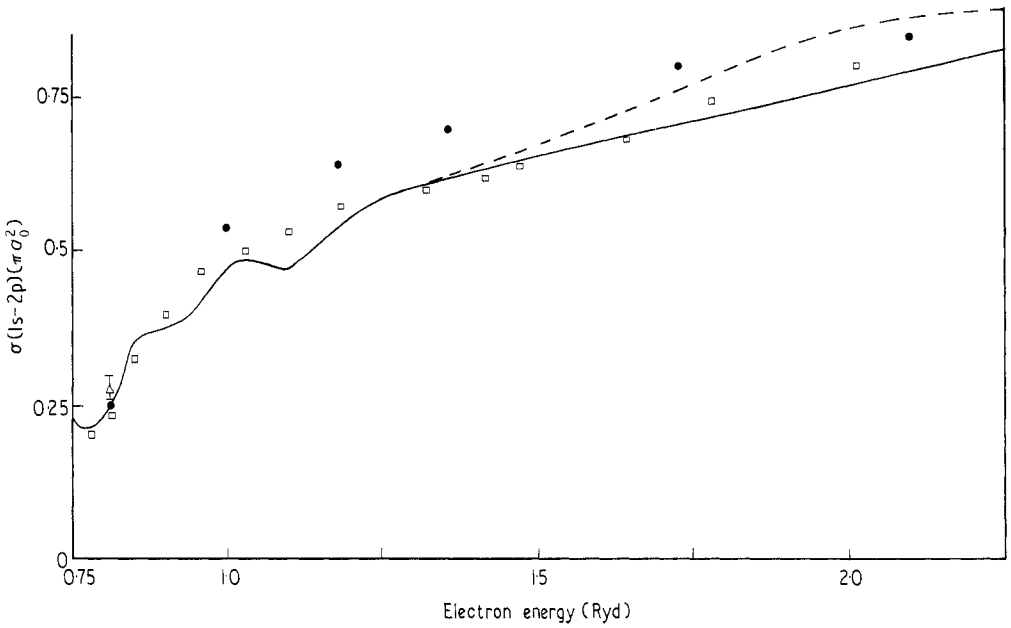

Figure 2. Total cross section (in units of πa_0^2) for

$$e + H(1s) \rightarrow e + H(2p).$$

As for figure 1, except that the experimental data shown are ⊼ Williams and Willis (1974), □ McGowan *et al* (1969) and ● Long *et al* (1968).

results, not shown here, which agree with those of Kochsmeider *et al*. For the 2p state, the data presented are the relative measurements of Long *et al* (1968), McGowan *et al* (1969), and the absolute results of Williams and Willis (1974).

The calculated 2s excitation cross sections agree rather well with the measurements of Kochsmeider *et al* which are normalized to the pseudostate calculation of Geltman and Burke (1970) in the range 10–12 eV between the $n = 2$ and $n = 3$ thresholds. Although our model is quite capable of predicting resonances, we have not attempted to investigate resonant structure below the $n = 3$ threshold in any detail. Our objective has been instead to determine the general behaviour of the cross section over a range of energies.

Some allowance for cascade effects involving the 3p state has to be made above the $n = 3$ threshold. We have followed the procedure of Kaupilla *et al* (1970) by adding $0{\cdot}23\ \sigma_{1s\rightarrow 3p}$ to the 1s–2s cross section in order to include cascade. The cross section for impact excitation of the 3p state has been obtained from the DWPO calculation of Syms *et al* (1975). When cascade effects are included, the calculated results are in rather good agreement with observation. For comparison, we have shown the results of the calculation of Burke and Webb using a smaller pseudostate basis, modified by including the same correction for cascade as applied to our results. Their calculated cross sections are also in good agreement with experiment after inclusion of the correction for cascade.

The calculated 2p excitation cross section is also in reasonably good agreement with experiment. In the 10–12 eV range, our results are in better accord with the measurements of Williams and Willis than with those of McGowen *et al*. Since the higher partial-wave cross sections calculated by the DWPO method are somewhat smaller than those obtained

in the Born exchange approximation, our calculated 1s–2p cross sections are somewhat lower than those obtained by Callaway and Wooten (1975) who used the Born exchange approximation to provide the high L correction. These differences increased with energy, and amount to about 13% at 30 eV ($\sigma = 0{\cdot}939\ \pi a_0^2$ if the Born correction is used, $0{\cdot}832$ if DWPO is employed). For comparison, one obtains $0{\cdot}948\ \pi a_0^2$ if the higher partial waves are taken from the published three-state close-coupling results of Burke *et al* (1963). The experimental results of Long *et al* and of McGowan *et al* (which are normalized to Long *et al*) tend to support the DWPO high L correction in comparison to that obtained from the Born exchange or three-state close-coupling approximations; however, if an experimental uncertainty of 10% is assumed, the preference is not strong. The present results (figure 2) agree with the experimental measurements of Long *et al* (1969), when normalized either to Williams and Willis (1974) at 11·02 eV, or to the DWPO calculations at 200 eV, to within the experimental error ($\pm 10\%$), throughout the energy range (10–200 eV).

We have attempted to estimate the total cross section for all scattering processes. The contributions from states $0 \leqslant L \leqslant 3$ can be obtained from the forward elastic scattering amplitude using the optical theorem. The elastic amplitude has been given by Callaway and Williams (1975). The contribution to the cross section from these values of L can be expressed, in view of the normalization conventions employed, by

$$\sigma_T = \frac{1}{k^2} \sum_S (2S+1) \sum_L (2L+1)\, \mathrm{Im}\, f_{L,S} \tag{3}$$

in which $f_{L,S}$ is the published scattering amplitude, and σ_T is in units of πa_0^2. We have supplemented the results obtained from (3) in the following way: (i) the contributions from $L \geqslant 4$ to the 1s–2p and 1s–3p cross sections have been added using the results obtained from the DWPO method, and (ii) a similar correction for $L \geqslant 4$ to the ionization cross section has been roughly estimated from the calculations of Burke and Taylor (1965) and Gallaher (1974). The results are shown graphically in figure 3, which compares the total cross section, σ_T, the elastic scattering cross section, σ_e, the cross section for the excitation of $n = 2$ states, σ_2, and the total inelastic cross section, σ_i. Specific resonance effects are not included; however, structure in the cross sections in the vicinity of the $n = 3$ and the ionization thresholds is obvious. Some of this may be due to pseudoresonances.

4. Differential cross sections and Lyα polarization

We have computed differential cross sections for the excitation of the 2s and 2p states using the procedure described in §2. The cross section for the excitation of the $n = 2$ states at an impact energy of $k^2 = 1{\cdot}21$ Ryd (16·46 eV) are shown in figure 4. Experimental results are not yet available in the energy range for which calculations are reported here.

The differential cross sections are more sensitive to the method used to include the large L contribution than are the total cross sections. For $k^2 = 2{\cdot}25$ Ryd (30·6 eV) our differential cross sections show oscillations which are apparently due to the mismatch in phase between the pseudostate and DWPO transition matrix elements. Unitarization of the results using Born K-matrix elements for the coupling terms ($L > 3$) has a significant smoothing effect at $k^2 = 2{\cdot}25$ and higher energies, and will be discussed elsewhere.

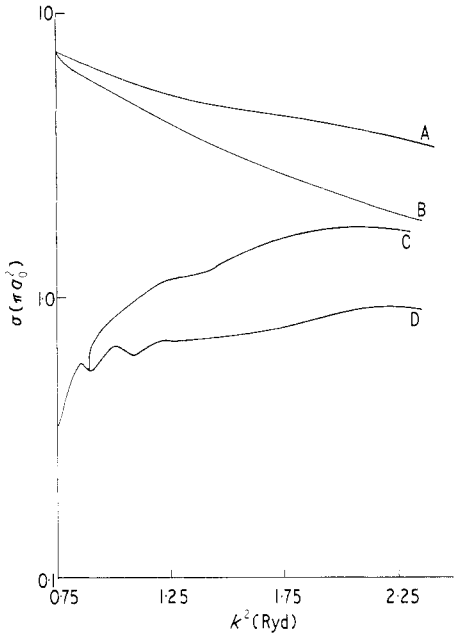

Figure 3. Calculated total cross sections, see text (units of πa_0^2). A, σ_T: cross section for all processes; B, σ_e: total elastic cross section; C, σ_i: total inelastic cross section; D, σ_2: total $n = 2$ cross section.

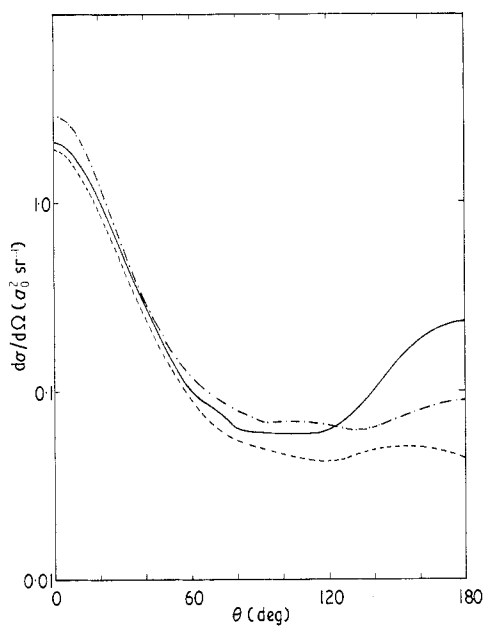

Figure 4. Calculated differential cross sections at 16·5 eV ($k^2 = 1{\cdot}21$), for

$$e + H(n = 1) \rightarrow e + H(n = 2)$$

in units of $a_0^2\,\mathrm{sr}^{-1}$. Full curve: total $n = 2$ cross section (present results); broken curve: 1s–2p cross section (present results); chain curve: 1s–2p cross section (Brandt and Truhlar 1974).

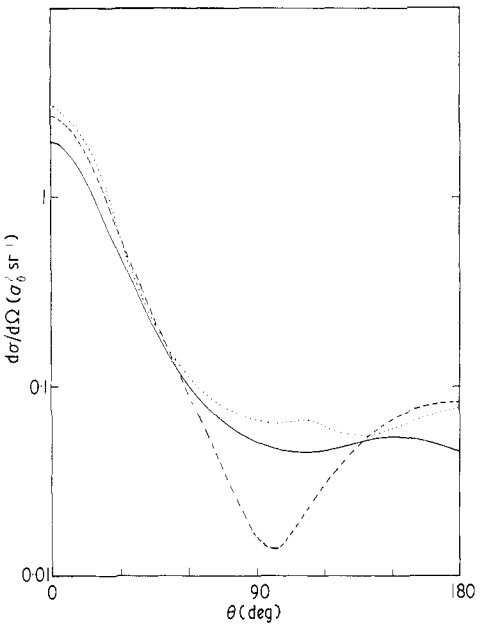

Figure 5. Calculated 1s → 2p differential cross section (in units of $a_0^2\,\mathrm{sr}^{-1}$, at $k^2 = 1{\cdot}21$. ————, present results (pseudostate $0 \leqslant L \leqslant 3$; DWPO II $L > 3$); · · · ·, Brandt and Truhlar (1974), six-state close-coupling; – – – – –, DWPO II (all L), McDowell *et al* 1975.

In figure 5 we compare the 1s → 2p differential cross section of the present work with the DWPO results of McDowell *et al* (1975) and the six-state close-coupling results of Brandt and Truhlar (1974), at an energy of 1·21 Ryd. The differences between the present results and the six-state close-coupling results are not large. However, the latter may overestimate the total cross section to some extent. It would appear to be difficult to distinguish close-coupling and distortion effects experimentally.

We have also computed the polarization, $P(90)$, of Lyα emitted following excitation of the 2p state at 90° to the incident beam, and our results are shown in figure 6, where they are compared with the experimental measurements of Ott *et al* (1970). At energies above 25 eV the present results agree with those obtained by McDowell *et al* (1975) in the DWPO II model, and with experiment. However we tend to slightly overestimate the observed values from 25 eV down to 12 eV, but the overall agreement with experiment now persists down to threshold. The effects of the spread in energy of the electron beam ($\simeq 0{\cdot}2$ eV) are appreciable at low energies and have not been included. The chain curve in figure 6 represents the close-coupling calculations of Burke *et al* (1968); the deviation from our results above $k^2 = 0{\cdot}86$ is due to resonance structure, which we did not examine explicitly.

5. Conclusions

A comparison of the present work with experiment shows that agreement within $\pm 10\%$ now exists from threshold to 30 eV, for total 1s–2s and 1s–2p cross sections.

Our calculated values for Lyα polarization also agree with experiment over this energy range, and this suggests that, at least in the neighbourhood of 90°, our predicted 2p differential cross sections should be reliable.

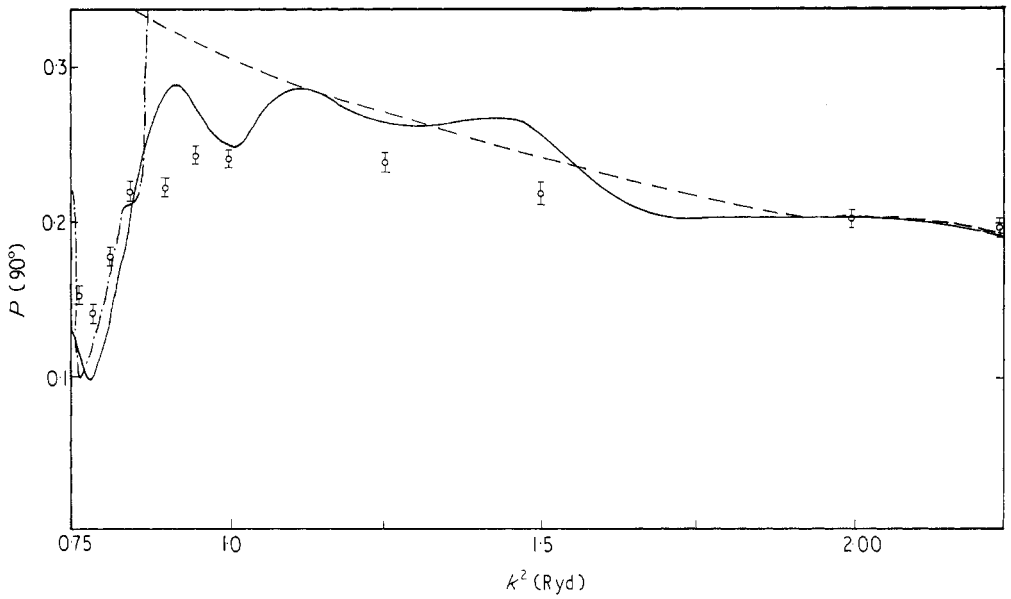

Figure 6. Polarization of Lyα at 90° to the incident beam. The experimental points are those of Ott *et al* (1970); ————, present results; – – – –, DWPO II (McDowell *et al* 1975); –·–·–·–·–, Burke *et al* (1968).

We believe that measurements of the differential cross sections for these processes in this energy range are now required.

The rather good agreement between the present results for the 1s → 2s and 1s → 2p total cross sections with those of Burke and Webb (1970), obtained using a five-state expansion, indicates that such pseudostate expansions may well be rapidly convergent The minor discrepancies between these calculations at energies below 1·5 Ryd is probably attributable to structure associated with the pseudostate thresholds.

Acknowledgments

We are indebted to Dr J W Wooten for assistance in the early phases of this work. One of us (JC) was an SRC Senior Visiting Fellow while engaged on this work.

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