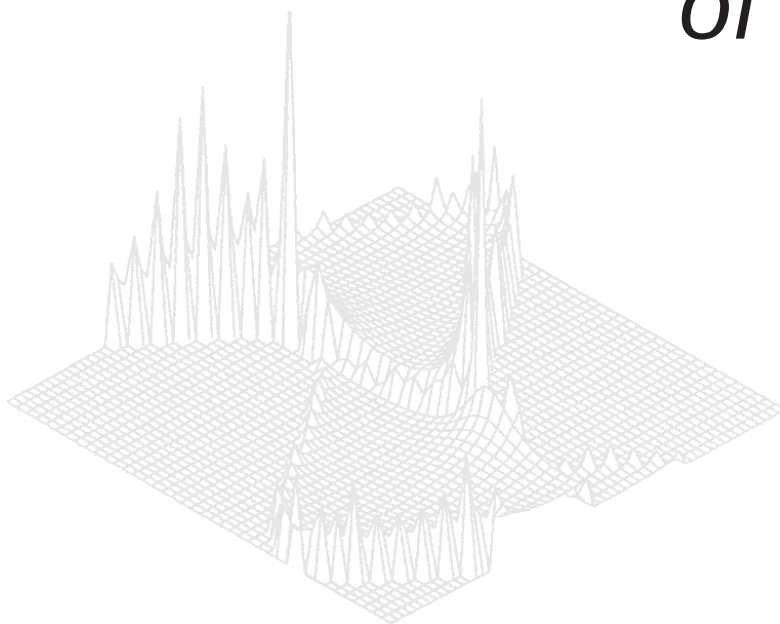

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New and Old Measurements of Electron Scattering in Atomic Hydrogen*

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Abstract

A critical look is made of discrepancies and agreements between new and old measurements and theories for elastic and $n = 2$ excitation of atomic hydrogen by electron impact, mainly at 16.5, 54 and 100 eV. A discussion of earlier work indicates the contributions of Weigold and colleagues. The difficulties of observing and modelling small scattered fluxes at backward scattering angles and of making absolute cross section calibrations are noted. New measurements of elastic scattering at 16.5 eV confirm earlier measured angular distributions. An absolute calibration of the differential cross section at 16.5 eV gives agreement within one standard deviation with intermediate energy R -matrix and multi-pseudostate close coupling values. At 16.5 eV, measurements of the separate 2s and 2p differential cross sections and the lambda, R and I correlation parameters again support the values from those theories.

1. Introduction

The central role of three-body Coulomb scattering in atomic physics has supported the continuing attention to electron scattering from atomic hydrogen. A major goal of theory has been a unified description of elastic, excitation and ionisation processes in atomic hydrogen and the subsequent prediction of scattering probabilities for other atoms and molecules. While there have been many theoretical studies of electron scattering, even from the earliest days of quantum mechanics, there have been few measurements particularly for atomic hydrogen. The present work examines some previous measurements and presents new measurements at 16.5 eV to guide theoretical methods. Also, on this occasion of celebrating Erich Weigold's sixtieth birthday, the significance and timeliness of the contributions of his group are acknowledged.

The contributions which set the scene for this paper on electron scattering from atomic hydrogen concern the theoretical advances by Madison *et al.* (1991) and Bray and Stelbovics (1992), the analyses of theory by van Wyngaarden and Walters (1986) and Scholz *et al.* (1991) and the comments by McConkey *et al.* (1988). The convergent close coupling method (Bray and Stelbovics 1992), the multi-pseudostate close coupling method (Wang *et al.* 1994), the intermediate energy R -matrix method (Scholz *et al.* 1991) and the exact second-order distorted wave method (Madison *et al.* 1991) have built on decades of advances in theoretical and computational methods. At about the same time these approaches have

* Dedicated to Professor Erich Weigold on the occasion of his sixtieth birthday.

realised the strengths of the perturbative Born and distorted wave approaches with second order exchange and of non-perturbative close coupling methods with pseudostate expansions to include continuum states. These methods have been applied with considerable success to a number of electron scattering processes in atomic hydrogen and, in general, for the processes and dynamical conditions to which they have been applied, obtain total and differential cross sections which agree within about 20% of one another. At energies within the range 20 to 50 eV for elastic and separate 2s and 2p excitations, the total and differential cross sections agree with one another and with measurement. The agreement with measurement at 35 and 54 eV for the angular correlation parameters is good at angles less than about 70° , but is not satisfactory at larger angles. It is not the purpose of this paper to discuss the theoretical models which has been done frequently, for example as referenced above. However, the values predicted by successful theory must, in principal, agree within several standard deviations of accurate observations which have been repeated in independent experiments. Only a few measurements are available and, when they have been repeated in independent laboratories, they tend to test experimental techniques and yield data with experimental uncertainties which are larger than required to guide theory. Some specific cases are discussed below. Attention is given to differential elastic and 2s and 2p excitation cross sections from a historical perspective and then subsequently to new measurements at 16.5 eV.

(1a) Elastic Differential Cross Sections (DCS)

To begin, a little of the history of these measurements is recalled. Prior to 1975 the pioneering work of Gilbody *et al.* (1961) at 3.4 eV, and nearby energies, showed a nearly isotropic angular distribution that was in marked disagreement with all theories. Their experiments and methods were state-of-the-art for that time and highly regarded. The advances of technology enabled a new apparatus (Williams 1975) to be designed initially for very low energies. Observations from 0.58 to 8.7 eV provided great detail to explore fully the partial wave analysis of the differential cross sections. The conclusions was readily reached that ‘exact’ variational, close-coupling and polarised orbital approximations gave excellent descriptions of the observations. Subsequently Shyn and Cho (1995) measured similar values within their larger experimental uncertainties for elastic DCSs at 5 and 7 eV, but their large angle data had noticeably higher values.

The success of this instrument led to further measurements in the near-threshold region from 10 to 30 eV reported in Callaway and Williams (1975) and, as shown in Figs 1 and 2 of their paper, there is good agreement between their pseudostate close coupling theory and measurement within experimental uncertainty. The limitations of that theory in handling the pseudostate expansion were not apparent at those low energies. The difficulties of the measurements and of making an absolute calibration of the angular distributions may be seen however. The differences between measurement and theory are generally within several standard deviations and become greater as the DCS decreases, at least for that particular apparatus and measurement techniques (Williams 1975; Williams and Willis 1975). But similar difficulties had appeared in the earlier elastic DCSs of Teubner *et al.* (1974) from 9.4 to 50 eV and of Lloyd *et al.* (1974) from 30 to 200 eV. Those data show more fluctuations in magnitude than the data of Williams and Willis

and have a larger (about 40%) normalisation uncertainty. Even more noticeably, later measured values, by Shyn and Cho (1995) at 30 eV and scattering angles larger than about 100° are considerably higher than earlier values.

Similar trends appeared in the 100 and 200 eV DCS of van Wingerden *et al.* (1977) where there are larger uncertainties and the relative values at larger angles differ from theory. At 200 eV van Wyngaarden and Walters (1986) claimed the best theory produced elastic DCSs that were probably accurate to 5% and consequently that the data of Williams and Willis (1975) seemed too high, particularly at 100 eV. However, the differences between their theory and those measured data varied only from 13% to 37%. Since one standard deviation experimental uncertainty was 10% to 15% over this range the difference between theory and measurement is within three standard deviations at most, and usually less than two standard deviations. That was not an unreasonable experimental uncertainty given the difficulty of the measurements and technology at that time. The current status at the energies selected to be in the low, intermediate and high energy regions is indicated in Fig. 1. At 16.5 eV the measured values reported by Callaway and Williams (1975) agree within small experimental uncertainties with the intermediate energy *R*-matrix values of Scholz *et al.* (1991) and the multi-pseudostate close coupling values of Wang *et al.* (1994). The relative accuracy and absolute calibrations of the measured data are consistent with theory. At 54 eV, the measured values of Williams and Willis (1975) are in good agreement with intermediate energy *R*-matrix values of Scholz *et al.* (1991) and the distorted wave second-order exchange values of Madison *et al.* (1991) and are about one standard deviation above the convergent close coupling values of Bray and Stelbovics (1992). At 100 eV the measured values are about one standard deviation uniformly above all the theoretical values which have merged to similar values. This suggests that an absolute calibration with improved accuracy is required if and when there is a need to test theory at that level. The calibration methods have been discussed, for example, by Lower *et al.* (1987).

(1b) $n = 2$ and Separate 2s and 2p DCSs

A brief history, including the contributions from Weigold and colleagues, of the $n = 2$ (i.e. summed 2s plus 2p) DCS and the separate 2s and 2p DCSs is again in order. The $n = 2$ excitation DCSs were measured from electron energy loss spectra at 13.9, 16.5 and 19.6 eV impact energies (Williams 1976). Multi-pseudostate close coupling values (Wang *et al.* 1994) at 16.5 eV are shown in Fig. 2 to be in excellent agreement with the measured values of Williams and Willis (1975). Similarly, good agreement between this theory and measurement was found for elastic scattering at this energy. At 54 eV the intermediate energy *R*-matrix values of Scholz *et al.* (1991) (calculated at 50 eV) and the distorted wave second-order exchange values of Madison *et al.* (1991) are in agreement within one standard deviation with measurement; however, the convergent close coupling values of Bray and Stelbovics (1992) are generally within two standard deviations of measurement. At 100 eV the experimental DCSs of Williams and Willis (1975) are supported by the data of Doering and Vaughan (1986) (not shown in the figure); the two data sets agree at large angles, within rather large error limits of about 30%, with the Doering and Vaughan results higher than those of Williams and Willis. The multi-pseudostate close coupling values of

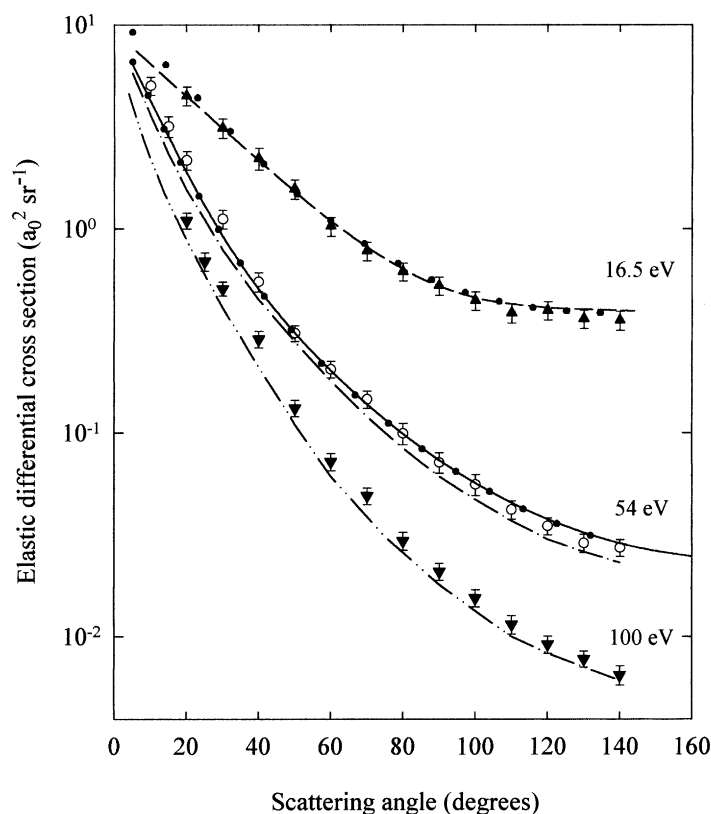


Fig. 1. Elastic differential cross sections for electrons scattered from atomic hydrogen. The measurements are at 16.5 eV [Callaway and Williams (1975) (triangles)], at 54 eV [Williams and Willis (1975) (open circles)] and at 100 eV [Williams and Willis (1975) (inverted triangles)]. Theoretical values are at 16.5 eV [Scholz *et al.* (1991) (dotted line) and Wang *et al.* (1994) (dashed line)], at 54 eV [Scholz *et al.* (1991) (dotted line), Madison *et al.* (1991) (full line) and Bray and Stelbovics (1992) (dot-dash line)] and at 100 eV [van Wyngaarden and Walters (1986) (dash-two-dot line)].

van Wyngaarden and Walters (1986) and the distorted wave second-order exchange values of Madison *et al.* (1991) (not shown in the figure for clarity) are in agreement with measurement at the smallest angles, but then become smaller than measurement as the scattering angle increases such that at 130° the data sets are about three standard deviations apart. It seems that the absolute calibration (for the 20° datum point) is adequate but the relative angular values decrease less rapidly than theory. A similar but less marked trend exists at 200 eV. It is pertinent here from the point of view of making accurate measurements to note that the theoretical values and the above measurements diverge when the DCS becomes less than about $0.07 \text{ a}_0^2 \text{ sr}^{-1}$. This difference gives an indication of the size of the spurious scattered signal which may be sought to identify the origin of the experimental high values.

An attempt to shed more light on such differences was made by Frost and Weigold (1980) who measured the ratios of the 2p and 2s excitations DCSs at

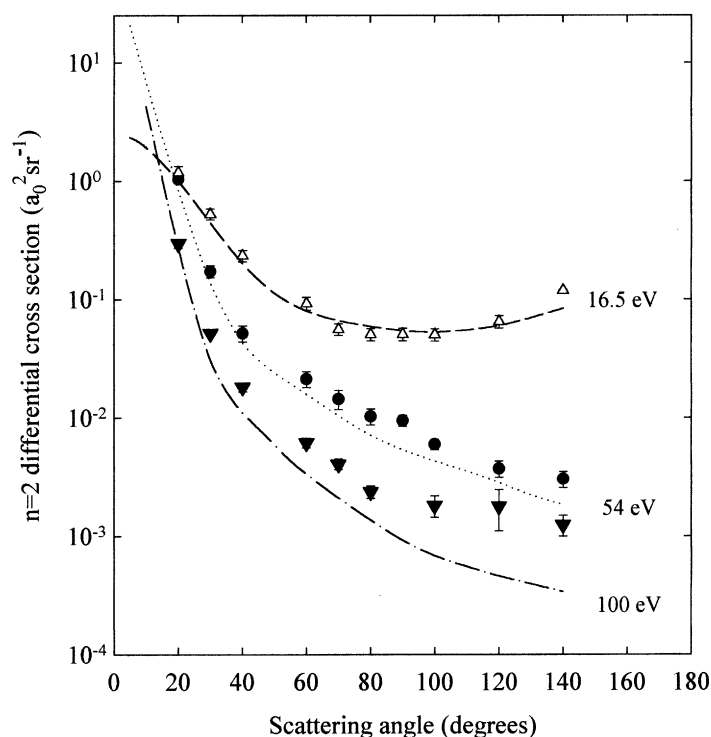


Fig. 2. Inelastic ($n = 2$ excitation) differential cross sections for 16.5, 54 and 100 eV electrons scattered from atomic hydrogen. The measurements by Williams and Willis (1975) are shown at 16.5 eV (open triangles), 54 eV (filled circles) and 100 eV (inverted triangles). The theoretical values are shown at 16.5 eV [Scholz *et al.* (1991) (dashed line)], at 54 eV [Bray and Stelbovics (1992) (dotted line)] and at 100 eV [van Wyngaarden and Walters (1986) (dash-dot line)].

54 eV from 10° to 130° . They used an electron-photon coincidence technique in which the ratio of the $n = 2$ energy loss electron count rate to the true coincidence rate was shown to be proportional to the ratio of the 2s to 2p DCSs. Consequently, the ratio would be independent of an absolute DCS calibration. At 54 eV, as shown in Fig. 3, their ratios are in agreement, within overlapping experimental uncertainty, with values by Williams (1981). However, at angles above about 70° the experimental uncertainty becomes large and both data sets become larger than the convergent close coupling ratios of Bray and Stelbovics (1992). Also it is about that scattering angle when the DCSs diverge. This observation suggests that, although absolute DCS calibration uncertainties are not present, both the ratio of the DCSs as well as the DCS values, still contain spurious signals perhaps with similar effects on the detected signals.

An attempt to resolve the discrepancy between theory and measurement was made by Lower *et al.* (1987) with measurements of the ratio of the elastic DCS to the (2s+2p) excitation DCS at 100 eV for 30° , 45° and 60° scattering angles. Their measured ratios differed from theory by 10% to 40% depending on angle and energy, while the experimental elastic DCSs deviated from theory by up to

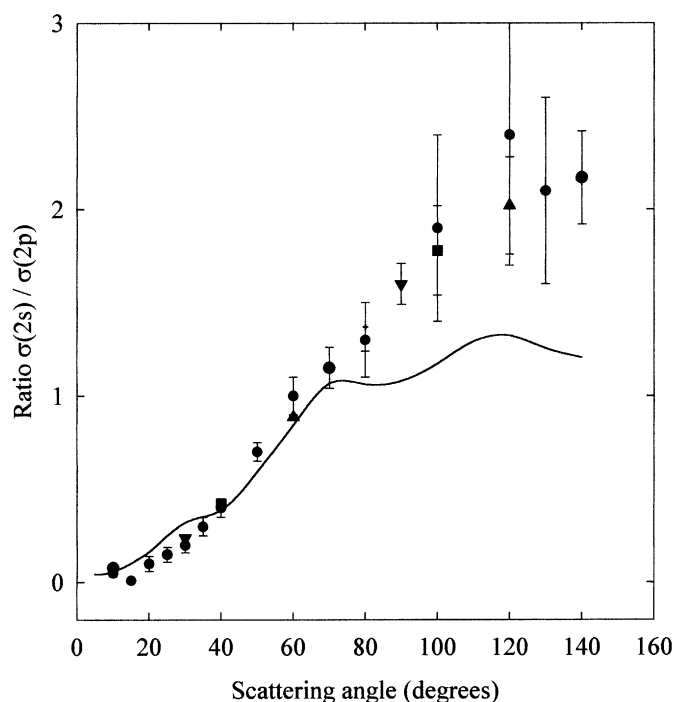


Fig. 3. Ratio of the 2s to 2p differential cross sections for 54 eV electrons incident on atomic hydrogen. The measurements are from Frost and Weigold (1980) (triangles) and Williams (1981) (closed circles). The line represents the convergent close coupling values (Bray and Stelbovics 1992).

20%. At angles above about 60° their measured ratios of the $n = 1$ to $n = 2$ DCS results are closer to the data of van Wingerden *et al.* (1977) rather than of Williams and Willis (1975) and so diverged further from the van Wyngaarden and Walters (1986) ‘twenty-pseudostate close-coupling’ calculated values. Both experiments used different calibration methods which added support to their values. This result widened the perceived difference between measurement and theory for which consistently lower values were obtained from various theories. Subsequent theories of Madison *et al.* (1991) and Bray *et al.* (1990) confirmed that the current theories obtained similar values at 100 eV. The measured values are judged to be in good agreement with theory at angles less than about 30° , but then diverge higher than the theory for larger scattering angles such that by 120° there is a difference of up to three standard deviations. The balance of the evidence is in favour of the theoretical values.

Measurement of the separate 2s and 2p DCSs is even more difficult, as indicated by Williams (1981), since each depends on coincident detection of the energy loss electron and the radiated 2p photon as opposed to just electron energy loss spectra for the $n = 2$ (summed 2s and 2p) DCS. At 54 eV, Fig. 4 shows the measured 2p DCS of Williams (1981) and the convergent close coupling (Bray and Stelbovics, 1992) and second-order distorted wave exchange values (Madison *et al.* 1991) are in good agreement at all angles. However, the measured 2s DCS becomes higher than theory for scattering angles greater than about 60°

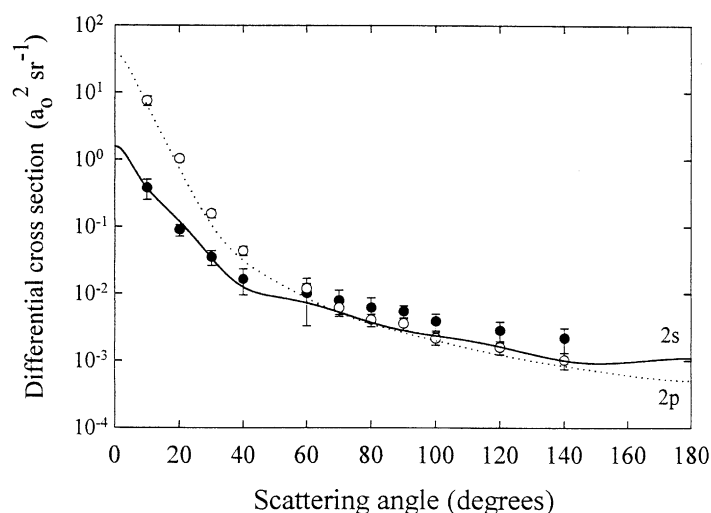


Fig. 4. Measured differential cross sections for excitation of the separate 2s and 2p states are shown for 54 eV electrons incident on atomic hydrogen. The measured values of Williams (1981) are the 2s DCS (filled circles) and 2p DCS (open circles) and the convergent close coupling values of Bray and Stelbovics are the 2s DCS (full line) for the 2p DCS (dotted line).

and differs by about two standard deviations at large angles. This region is also approximately where the $n = 2$ DCSs and the ratio of the 2s to 2p DCSs becomes larger than theory and strongly suggests that the measurements involving the 2s state require further study.

The interest in the 54 eV scattering has been motivated in part by the differences in angular correlation parameters from theory and measurement and perhaps not revealed where measurements should be made to obtain more evidence of the reliability of an apparatus and of more accurate measurements of the 2s and 2p DCSs. Fig. 5 shows the DCSs for the separate 2s and 2p excitations at 16.5, 54 and 100 eV calculated by the pseudostate close coupling method (Wang *et al.* 1994), the convergent close coupling method (Bray and Stelbovics 1992) and the twenty-pseudostate close coupling method (van Wyngaarden and Walters 1986), respectively. It is clear that measurements at 16.5 eV, rather than 54 or 100 eV, and particularly near 60°, offer better prospects for obtaining accurate 2p DCSs and for determining if scattered electrons from the 2s state cause experimental problems.

Finally, just above the $n = 2$ excitation threshold, the integrated cross sections for the separate 2s and 2p state agree within experimental uncertainty with the theoretical values from the convergent close-coupling, the intermediate-energy R -matrix, the convergent J -matrix and a pseudostate calculation (as discussed by Bray *et al.* 1996). Such a result is expected for these methods since they converge to the exact values. Similarly the measured elastic and $n = 2$ DCSs at 16.5 eV are in agreement with the intermediate energy R -matrix values so the new measurements of this paper of the separate 2s and 2p DCSs at 16.5 eV were expected to be a good test of the finer features of those theories.

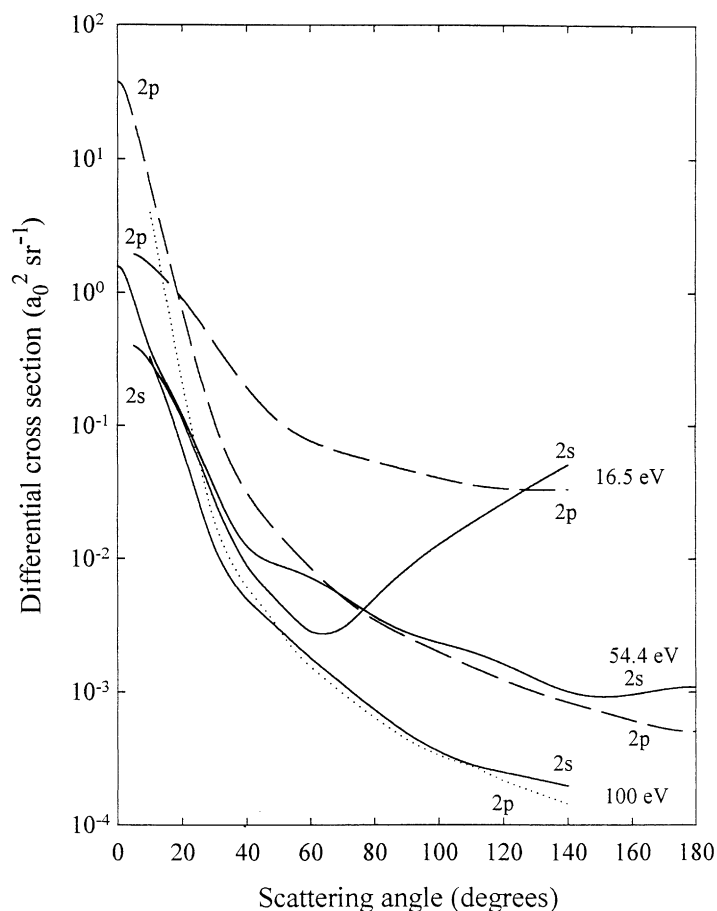


Fig. 5. Theoretical 2s (full line) and 2p differential cross sections for 16.5 eV (dashed line), 54 eV (dashed line) and 100 eV (dotted line) electrons incident on atomic hydrogen. The 16.5 eV data are from Wang *et al.* (1994), the 54 eV data from Bray and Stelbovics (1992) and the 100 eV data from van Wyngaarden and Walters (1986).

2. Experimental Method and Apparatus

The experimental apparatus is basically similar to that used in similar earlier studies (Williams and Willis 1975; Williams 1975, 1981). The electron energy analysers and optics have the same design as used previously, however, improvements have reduced the filling factors of the lenses, reduced electron scattering from surfaces and reduced potential sources of spurious signals. The polarisation analysis has changed from reflective gold surfaces to transmission quarter-wave plates of magnesium fluoride. Details of this type of polariser and its calibration are given by Uhrig *et al.* (1994).

Radiation trapping effects were found to influence the data in a way similar to that shown previously (Williams *et al.* 1992; Mikosza *et al.* 1994) for 58.4 nm radiation from helium. In summary, the excited state lifetime, which can be

measured an order of magnitude more quickly than the state parameters, reflects the relaxation rates and was shown to be a sensitive detector of radiation trapping. The present correlation measurements were made at a beam density sufficiently small that radiation trapping effects were not detectable in the 2p lifetime measured using the radiated circularly polarised photon signal. These results are being reported separately.

3. Results

Elastic angular distributions have been measured at 16.5 eV for angles from 10° to 140°. The relative values are not discernibly different from the data reported by Callaway and Williams (1975) shown in Fig. 1 and so are not indicated in the figure. The present data were made absolute by the same procedure used by Williams and Willis (1975). Helium was mixed with the hydrogen and then measurements were made of the ratio of atomic hydrogen to helium elastic DCSs at 16.5 eV. The resonance characteristics at 19.3 eV in the elastic channel were determined and a phase shift analysis at that and lower energies enabled an absolute cross section to be determined.

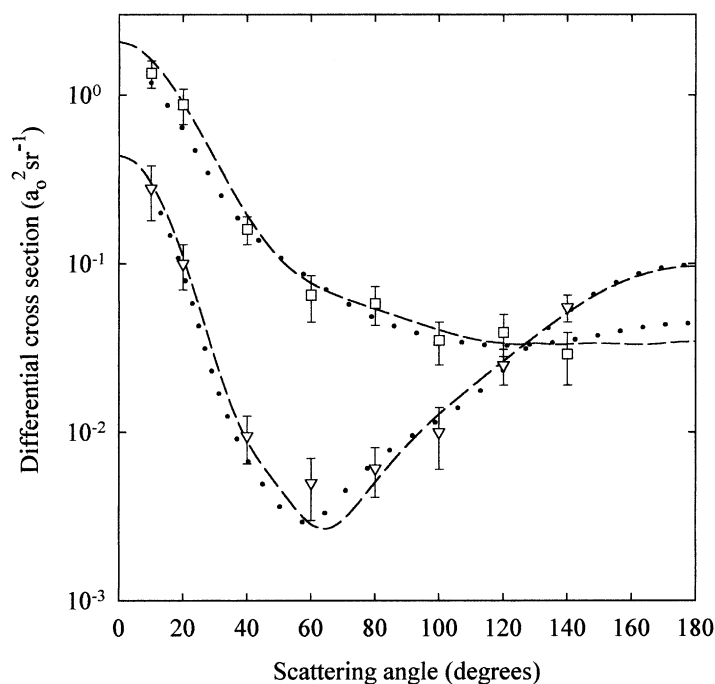


Fig. 6. Present measurements of the 2s (inverted triangles) and 2p (squares) differential cross sections for 16.5 eV electrons incident on atomic hydrogen as a function of electron scattering angle. The pseudostate convergent close coupling values (Wang *et al.* 1994) are shown as dashed lines and the intermediate energy close coupling data (Scholz *et al.* 1991) as dotted lines.

The separate 2s and 2p differential cross sections at 16.5 eV have been measured using the method (Frost and Weigold 1980; Williams 1981) of coincidence detection of the Lyman-alpha photon and the 10.2 eV energy loss electrons. Fig. 6 shows that the measured values are in agreement within the experimental uncertainty with the intermediate energy R -matrix values (Scholz *et al.* 1991) and the pseudostate close coupling values (Wang *et al.* 1994). As indicated in Fig. 2 for the $n = 2$ differential cross section both theories give values in agreement with measured values within experimental uncertainty. Also the former method gave good agreement with the total 2s and total 2p cross sections in the energy region near threshold (Bray *et al.* 1996).

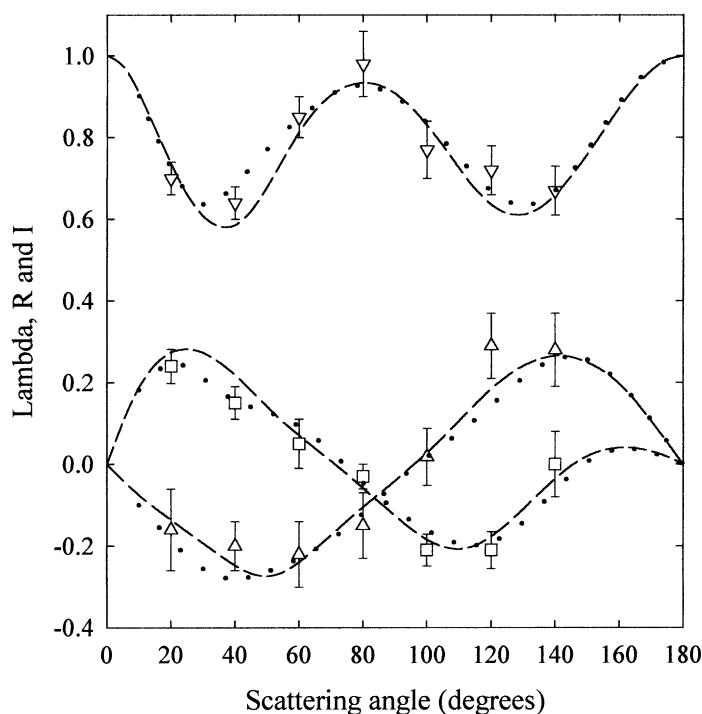


Fig. 7. Values of the lambda, R and I parameters are shown as a function of the electron scattering angle for an incident electron energy of 16.5 eV. The measured values are shown as lambda (inverted triangles), R (squares) and I (triangles). Other symbols are as for Fig. 6.

To complete the description of the 2p state, and so obtain a complete and consistent data set at 16.5 eV, the correlation parameters lambda, R and I were measured. Both angular and polarisation correlation methods were used to obtain the measured values shown in Fig. 7. The values of all three parameters are in agreement, within the experimental uncertainties, with the pseudostate close coupling values (Wang *et al.* 1994) and the intermediate energy R -matrix values (Scholz *et al.* 1991). The good agreement is in marked contrast with earlier differences between theory and measurement of these parameters at 54 eV. Here the angular dependence of all three parameters shows a tendency towards a

simplified sinusoidal form which reflects the relative size of the state multipoles near threshold, the subsequent simplification of the sinusoidal expressions for the state multipoles and the dominance of terms in either θ or 2θ , where θ is the scattering angle. The R and I parameters have opposite signs and the R parameter shows negative values at large scattering angles.

4. Conclusion

The present measurements at 16.5 eV for elastic and $n = 2$ differential cross sections, as well as the separate 2s and 2p differential cross sections and the lambda, R and I correlation parameters, present an internally consistent set of data. They are in agreement with values from the intermediate energy R -matrix method of Scholz *et al.* (1991) and the pseudostate close coupling method of Wang *et al.* (1994). Similar measurements are in progress for 54 eV where Salim *et al.* (1997) and O'Neill *et al.* (1998) have indicated progress.

Acknowledgments

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