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Principal Quantum Number Dependence for Electron–Hydrogen Collisions*

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Abstract

Over the last two decades, there has been considerable interest in the electron–atom scattering problem. Most of this work has concentrated on elastic scattering and excitation of the lowest energy states. However, due to recent technological advances, it is now becoming possible to examine experimentally the excitation of higher lying states. The important question then concerns whether these higher states contain new information. It has been argued that the scattering amplitudes for electron–helium excitation should scale with principal quantum and thus contain no new information. The purpose of this work is to examine the n-dependence for electron–hydrogen scattering. The converged-close-coupling and second-order distorted-wave methods have been used to calculate scattering amplitudes for excitation of the $n = 2$, 3 and 4 levels of the hydrogen atom. The n-dependence of the integrated cross sections, differential cross sections and angular correlation parameters will be discussed for energies from threshold to 500 eV.

1. Introduction

In the past decade there has been significant progress in the area of electron–atom collisions both experimentally and theoretically. On the experimental side, electron–photon coincidence measurements have now been carried out for excitation of the lowest energy states of hydrogen, the alkali atoms, the inert gases, and even of some of the heavier elements. For a review of this work, see Andersen *et al.* (1988). With the technological advances of the last few years, it is now becoming possible to examine the excitation of the higher lying states of various targets. The important question then is what new information can be learned from studying the higher energy states?

Csanak and Cartwright (1986) addressed this question for electron excitation of helium. They concluded that for energies above the ionisation threshold, the primary n-dependence for the T-matrix can be factored out. This implies that differential and integral cross sections for any n level can be obtained from lower lying states using a scaling formula. Further, ratios of the various magnetic sublevel T-matrices would be independent of the principal quantum number n

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and as a result the measured correlation and coherence parameters would be n-independent. In short, if the n-dependence for the T-matrix can be factored out, then there is little new information to be learned from studying the higher n levels. Consequently, this is a very important issue.

The purpose of this paper is to investigate the n-dependence of the correlation parameters, the differential cross section (DCS), and the integrated cross sections (ICS) for excitation of the 2p, 3p and 4p states of hydrogen in the energy range from 20 to 500 eV.

2. Scaleability of the Wavefunctions

The essence of the scaleability argument is that the scattering is controlled by the region of space close to the nucleus where the ground-state wavefunction is non-zero. Within this region, wavefunctions for fixed angular momentum and increasing principal quantum number tend to be approximately scaleable. Since the T-matrix involves integrals of these wavefunctions, scaleability of wavefunctions translates directly into scaleability of the T-matrix for this region (Csanak and Cartwright 1986).

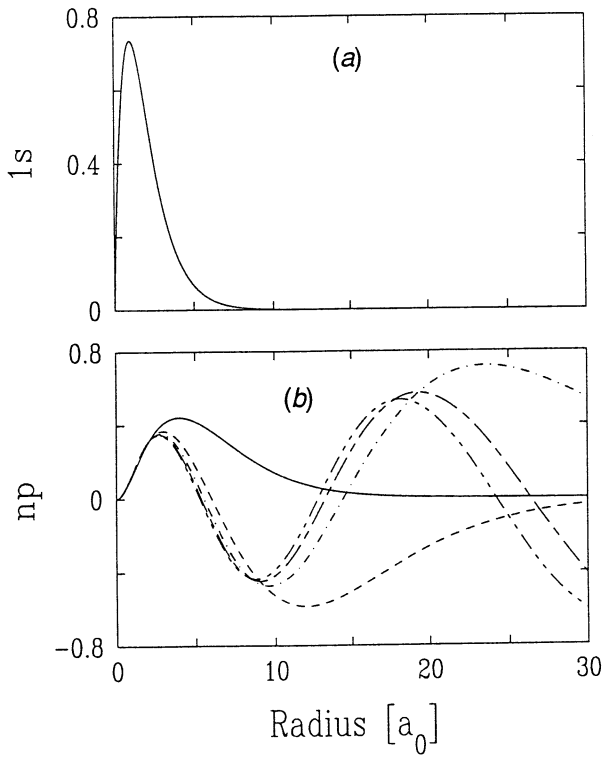

Fig. 1. A comparison of scaled hydrogen wavefunctions, (*a*) the 1s wavefunction and (*b*) the 2p to 6p wavefunctions, are displayed multiplied by the scale factor $(n/2)^{-3/2}$. The scaled p-state wavefunctions are as follows: solid curve, 2p; short-dash curve, 3p; dot–dash curve, 4p; short-dash–long-dash curve, 5p; and two-short-one-long-dash curve, 6p.

This scaleability of wavefunctions is demonstrated in Fig. 1 for hydrogen. The ground state for hydrogen is displayed in (*a*). Quantum-defect theory (Seaton 1983) predicts that the scaling factor for small radius and increasing principal quantum number n should be proportional to $n^{-3/2}$. Consequently, in (*b*) the 2p, 3p, 4p, 5p and 6p orbitals are shown scaled to the 2p state with the factor $(n/2)^{-3/2}$. It is seen that all the np orbitals are indeed approximately scaleable for small r and the scaleability becomes even better as the principal quantum number increases. Interestingly, the scaled 3p through 6p orbitals of hydrogen are very similar out to a distance of about 10 atomic units.

The Csanak and Cartwright argument applied to hydrogen would then suggest that only the region less than about 6 atomic units is important. However, it is known that the outer region can also be very important. For example, in a first-order perturbation theory, the exchange amplitude can depend significantly on more distant collisions and the exchange amplitude plays an important role for low-to-intermediate-energy collisions (Madison *et al.* 1991). Moreover, the outer region is certainly important for higher order terms in a perturbation series and it is also known (Madison *et al.* 1991) that these terms are very important. Consequently, it would be logical to conclude that although the approximate scaling of wavefunctions for small radii is interesting, physical observables would probably not scale with principal quantum number.

3. Theories

In 1986, the scaleability ideas were tested using first-order theories. In the last few years, the availability of new extremely fast electronic computers has enabled theoreticians to develop significantly better models which have produced a much improved description of electron–atom scattering. Two of these methods, the converged-close-coupling (CCC) (Bray and Stelbovics 1992) and the second-order distorted-wave (DWB2) (Madison *et al.* 1991) have been shown to predict reliable results for electron–hydrogen scattering. We use both of these theories to examine the n-dependence for electron–hydrogen scattering. The interested reader may find a detailed description of the two theories in the original publications. In brief, the idea of the CCC method is to expand the quantum mechanical wavefunction for the system in terms of a subset of a complete basis set for the one-electron Hamiltonian and then increase the number of terms in the subset expansion until a desired convergence is achieved. For the case of the DWB2, the first two terms of the distorted-wave perturbation series are evaluated without making approximations (other than numerical). For the case of the second-order term, the coupling to all discrete and continuum intermediate states is summed and integrated to numerical convergence. The DWB2 neglects third and higher order terms which means that it is an intermediate to high-energy approximation. It has been shown that third and higher order terms are not important for electron–hydrogen scattering for incident electron energies greater than about 30–50 eV.

4. Results

(*4a*) *Angular Correlation* (λ)

The angular correlation parameters can be obtained from the amplitudes A_m for excitation of the np_m substates. Here n is the principal quantum number for

a p state and m denotes the magnetic sublevel ($m = -1, 0, 1$). Although there are a number of different parameters which can be presented, they all depend on ratios of amplitudes. Here we will examine one of the common ones, namely the relative probability for exciting the $m = 0$ sublevel 1, which is defined by

$$\lambda = \frac{a_0\, a_0^*}{a_0\, a_0^* + 2a_1 a_1^*} \,. \tag{1}$$

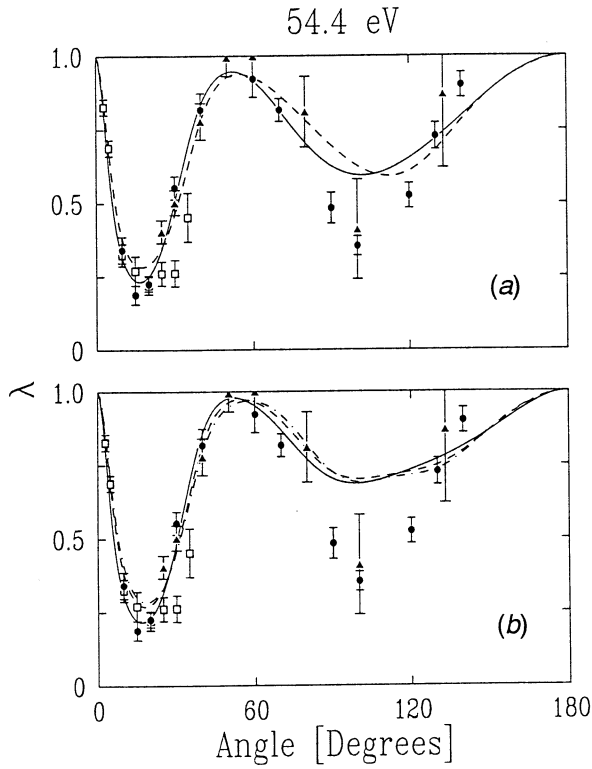

Fig. 2. The λ-parameter for excitation of 2p, 3p and 4p states of hydrogen: (a) contains the DWB2 results and (b) the CCC results. The theoretical curves are as follows: solid curve, 2p state; short-dash curve, 3p state; and dot–dash curve, 4p state. The 2p experimental data are: filled circles, Williams (1981); filled triangles, Weigold *et al.* (1980). The open boxes are the 3p results of Williams *et al.* (1993).

The most complete set of studies for the λ parameter has been performed for an incident electron energy of 54·4 eV. DWB2 and CCC results for the λ parameter are presented in Fig. 2 for excitation of the 2p, 3p and 4p states of hydrogen. Fig. 2a contains the DWB2 results and Fig. 2b the CCC results. The experimental data are the same in both and the horizontal axis is the scattering angle for the projectile electron after the collision. Filled experimental data points are for excitation of the 2p state and the open squares are for excitation of the 3p state. Both theoretical calculations predict λ parameters that are the

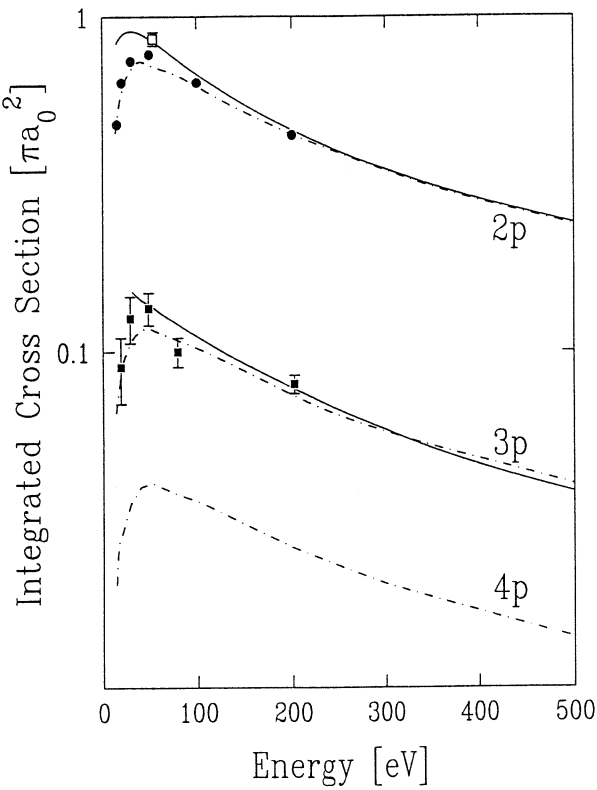

Fig. 3. Integrated cross sections for electron excitation of the 2p, 3p and 4p states of hydrogen. The theoretical curves are: solid curve, DWB2; dot–dash curve, CCC. The experimental results are: solid circles, recommended values of Trajmar and Kanik (1994); open square, integrated DCS of Williams (1981); and filled squares, measurements of Mahan *et al.* (1976).

same to within the experimental error for all principal quantum numbers n. It should also be noted that the DWB2 and CCC results are nearly identical except that the DWB2 minimum near 110° is slightly deeper and closer to the experimental data. In the case of the experimental data, the 3p results have overlapping error bars with the 2p results for most of the measured points.

In the beginning of this work, we believed that a simple scaling for T-matrix amplitudes must be wrong since we knew that accurate calculations had to be extended to a radius of about 100 a_0 (far beyond the region where scaling of the wavefunctions is reasonable). However, Fig. 2 indicates that in spite of all the experimental and theoretical efforts to measure and calculate the high n-level results, the answer is essentially independent of n. Bubelev *et al.* (1995) have examined other incident electron energies and other angular correlation parameters and they arrived at the same conclusion. Consequently, it appears that there is no new physics to be learned from looking at higher n, at least as far as the angular correlation parameters are concerned.

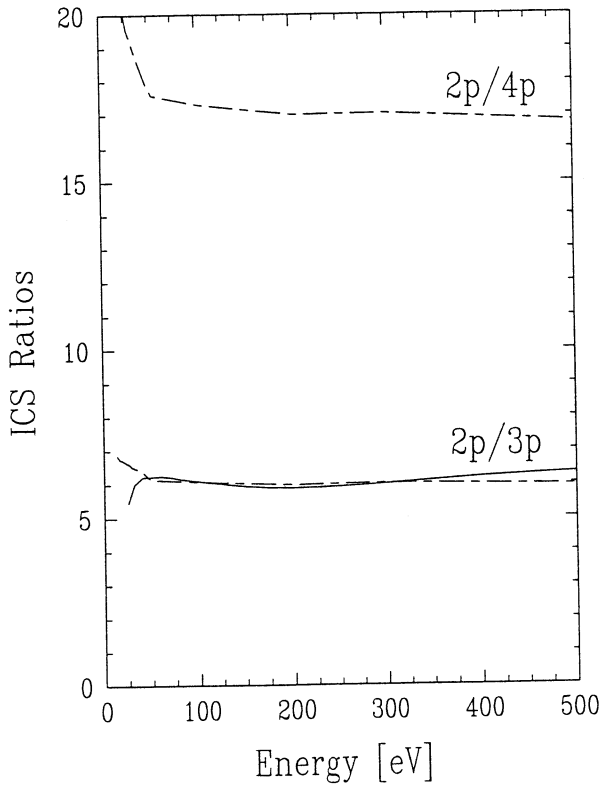

Fig. 4. Ratios of integrated cross sections. The theoretical results are: solid curve, DWB2; dashed curve, CCC.

(*4b*) *Integrated Cross Sections*

Recently there has been considerable interest in integrated cross sections (ICS) for electron scattering from hydrogen (Trajmar and Kanik 1995). Experiments are currently in progress at JPL to measure the polarisation fractions and integrated cross sections for exciting the 2p, 3p and 4p levels of hydrogen (Slevin 1994). Therefore, it would be interesting to see if the integrated cross sections exhibit a scaleability.

The integrated cross sections for excitation of the 2p and 3p levels of the hydrogen atom are shown in Fig. 3. The filled circles are the recommended values of Trajmar and Kanik (1995) for excitation of the 2p state. These values were obtained from a critical review of all the existing experimental data for integrated cross sections. The open square for 2p excitation is the result of integrating the experimental differential cross sections at 54·4 eV of Williams (1981). Both the DWB2 and CCC are in reasonable agreement with the experimental data. It is clear that the shapes of the ICS for different n levels look similar particularly for the higher energies.

To check for scaleability of the ICS, one needs to look at the ratios of the ICS for different n levels. These ratios are shown in Fig. 4 for both the DWB2 and

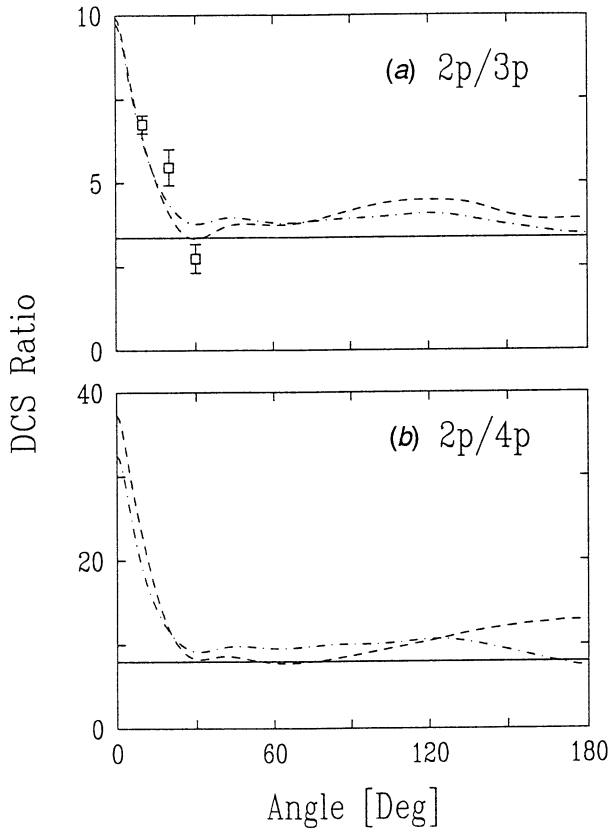

Fig. 5. Ratios of differential cross sections for an incident electron energy of 54·4 eV. The theoretical results are: dashed curve, DWB2; dot–dash curve, CCC. The solid line in each figure represents the prediction of n^{-3} scaling. The open squares are ratios obtained from the measurements of Williams (1981) and Williams *et al.* (1993).

CCC. For energies below 50 eV, the theoretical ratios are not constant. However, above 50 eV, the ICS ratios are relatively constant. Interestingly, however, the constant is significantly different from that predicted by n^{-3} scaling. If one assumes that the ICSs scale as n^{-x}, then the approximate value of x which we obtain from the theoretical results are as follows: for 2p/3p, x = 4·4; and for 2p/4p, x= 4·1. It can be argued that for very large n, the cross sections must scale as n^{-3}. Although, the theoretically predicted exponents are decreasing with n, it is clear that the lower n values differ significantly from the expected scaling.

(*4c*) *Differential Cross Sections*

The ratio of the DCS for an incident electron energy of 54·4 eV is presented in Fig. 5. The experimental ratio of 2p/3p was calculated from the measurements of Williams (1981) and Williams *et al.* (1993). The horizontal line in each plot is the constant predicted by n^{-3} scaling. Although the small angle DCS contains no indication of being scaleable either theoretically or experimentally, for large

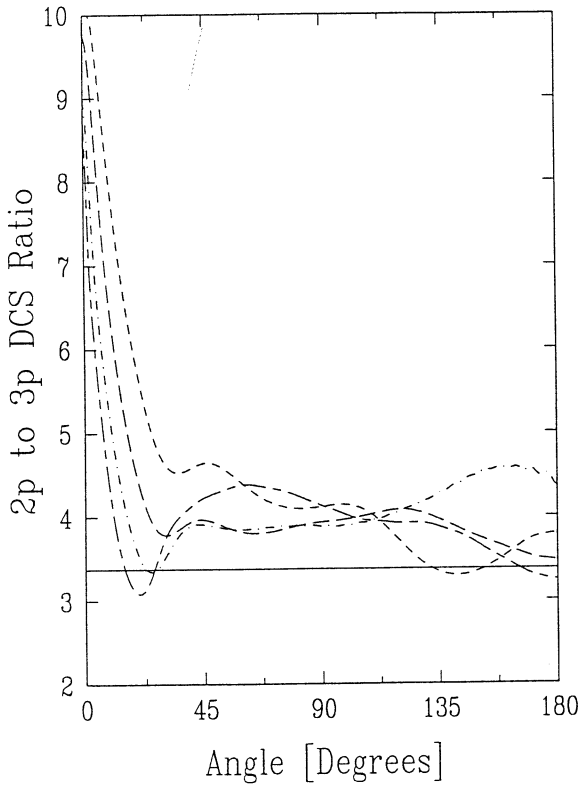

Fig. 6. Energy dependence of the ratio of 2p/3p differential cross sections. The energies of the theoretical CCC results are: small-dash curve, 35 eV; long-dash curve, 54·4 eV; dot–dash curve, 100 eV; and long-dash-short-dash curve, 200 eV. The solid line represents the prediction of n^{-3} scaling.

scattering angles the ratios are relatively flat and approximately that predicted by the n^{-3} scaling rule.

The large angle behaviour can be understood as follows. To be scattered into a large angle requires a close collision with the nucleus. As a result, large scattering angles correspond to collisions that take place predominantly within the 1s orbital. From Fig. 1, it is seen that within this region the wavefunctions are approximately scaleable and as a result the cross sections would be expected to scale approximately as n^{-3}. The fact that the ratios deviate from that predicted by n^{-3} scaling indicates that the outer region cannot be neglected even for hard collisions.

The energy dependence of the 2p/3p ratio is presented in Fig. 6. The solid line at the constant ratio value of 3·4 is the n^{-3} scaling prediction. It is clear that the small angle DCS shows no indication of obeying a scaling law at any of these energies. When one considers the fact that the small angle DCS determines the ICS, these results would appear to contradict the results presented in Fig. 4. It is very peculiar that the small angle DCS is not scaleable and yet the ICS apparently are. So far, we have not found a simple explanation for this

phenomenon. For the larger scattering angles, there is no systematic tendency to approach the n^{-3} scaling with increasing energy as found for the λ parameter.

5. Conclusion

We have performed second-order DWB2 and converged-close-coupling (CCC) calculations for the 2p, 3p and 4p excitation of atomic hydrogen and investigated the n-dependence of the λ parameter, the integrated cross section, and the differential cross section. Although the theoretical results do not support the simple predictions of an n^{-3} scaling, many features of this model were found. For example, it was found that the λ parameter is nearly n-independent for intermediate to high energies and depends only slightly on the principal quantum number n at low energies. Ratios of integrated cross sections were approximately constant for intermediate to high energy but the ratio was significantly different from that predicted by the n^{-3} rule. Differential cross sections do not even approximately scale with the principal quantum number for small and intermediate angles. On the other hand, the DCS do scale approximately as n^{-3} for large scattering angles. Unlike the λ parameter, the DCS does not approximate the scaling law better with increasing energy.

The final conclusion of this study is that for increasing n, the most interesting 'new' information is contained in the small angle DCS.

Acknowledgments

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