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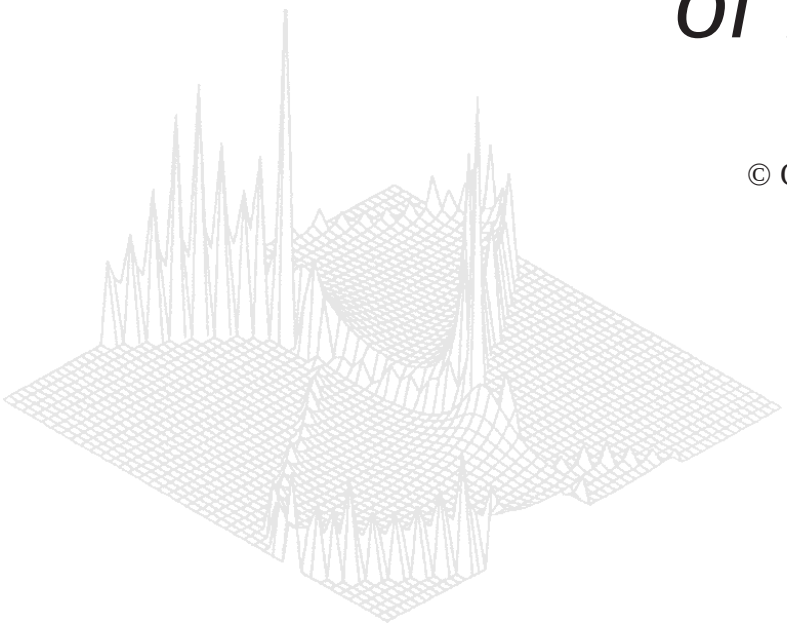

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Electron-impact Ionisation of Atomic Hydrogen from Near Threshold to High Energies

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Abstract

Application of the convergent close-coupling (CCC) method to electron-impact ionisation of the ground state of atomic hydrogen is considered at incident energies of 15·6, 17·6, 20, 25, 27·2, 30, 54·4, 150 and 250 eV. Total through to fully differential cross sections are presented. Following the analysis of Stelbovics (1999) the equal-energy sharing cross sections are calculated using a solely coherent combination of total-spin-dependent ionisation amplitudes, which are found to be simply a factor of two greater than the incoherent combination suggested by Bray and Fursa (1996). As a consequence, the CCC theory is particularly well-suited to the equal-energy-sharing kinematical region, where it is able to obtain convergent absolute scattering amplitudes, fully ab initio. This is consistent with the step-function hypothesis of Bray (1997), and indicates that at equal-energy-sharing the CCC amplitudes converge to half the step size. Comparison with experiment is satisfactory in some cases and substantial discrepancies are identified in others. The discrepancies are generally unpredictable and some internal inconsistencies in the experimental data are identified. Accordingly, new (e, 2e) measurements are requested.

1. Introduction

Our primary motivation in the study of electron–atom interactions is to provide accurate data for the needs of science and industry. To this end the primary emphasis of our study has been on discrete excitation processes. The locally developed convergent close-coupling (CCC) method was aimed at resolving the long-standing discrepancy of the elementary electron-impact 2P excitation in atomic hydrogen (Bray and Stelbovics 1992). The basic idea was the same as used earlier in, for example, the pseudostate close-coupling method of van Wyngaarden and Walters (1986), except that the generation of the pseudostates was done using an orthogonal Laguerre basis. This allowed for a systematic study of convergence in the observable of interest (e.g. 2P excitation) with increasing number of states N. The association of the pseudostates with an equivalent quadrature rule for the infinite sum and integral over the true target discrete and continuum spectrum indicated the importance of an efficient numerical implementation that allowed for coupling of as many states as possible for given computational resources.

Our interest in ionisation has come about rather indirectly. First we noted that the CCC method was able to reproduce the total e–H ionisation cross section (Bray and Stelbovics 1993). This cross section was obtained by essentially summing the

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cross sections for excitation of the positive-energy pseudostates, thereby identifying excitation of these states with ionisation processes. Another important indication that the CCC method, and close-coupling approaches generally, should be able to obtain accurate ionisation cross sections was found by application to 3P excitation of sodium (Bray 1994*a*). It was found that in order to be certain of obtaining accurate scattering amplitudes, for even the sodium 3P excitation, coupling within the ionisation channels had to be treated accurately. This was a most unexpected result with the consequence of our direct interest in ionisation processes.

In recent years considerable progress has been made in the ability of theory to reproduce fully differential measurements of atomic electron-impact ionisation. There are a number of theoretical approaches. Some approach the problem from the asymptotically correct three-body boundary conditions (Brauner *et al.* 1989, 1991*a*; Berakdar and Briggs 1994; Berakdar 1997; Chen *et al.* 1998; Jones and Madison 1998). Others are based on the Born approximation with the introduction of distorting and other potentials to improve the accuracy at lower energies (Pan and Starace 1991, 1992; Jones *et al.* 1992; Whelan *et al.* 1993, 1994; Röder *et al.* 1996*c*). More recently, a new and very promising development involves evaluation of ionisation without reference to asymptotic boundary conditions (McCurdy *et al.* 1997; Baertschy *et al.* 1999). There are also time-dependent approaches (Ihra *et al.* 1995; Pindzola and Schultz 1996). Another approach attempts to solve the Schrödinger equation of the scattering system subject to the approximation that the total wave function is expanded in a finite set of square-integrable target states (Curran and Walters 1987; Curran *et al.* 1991; Bray *et al.* 1994). It is the latter approach that is of particular interest to us. It allows for the treatment of discrete excitation and ionisation simultaneously, which to our mind is necessary to be sure of the accuracy of either calculation.

The CCC theory has been extensively applied to e–He ionisation at high (Bray and Fursa 1996*a*), intermediate (Röder *et al.* 1996*a*, 1996*b*; Bray *et al.* 1997; Rioual *et al.* 1998) and low (Bray *et al.* 1998) energies. Most encouraging was the ability to accurately describe both excitation and ionisation 100 eV data using a single CCC calculation (Bray and Fursa 1996*a*). During the course of this study some difficulties relating to the accuracy of absolute differential ionisation cross sections were identified and studied systematically (Röder *et al.* 1997*a*). It was determined that with decreasing projectile energy the singly differential cross section (SDCS) develops unphysical oscillations, which in turn affect the magnitude of the angle-differential ionisation cross sections, though apparently not their angular distributions. The source of this problem was suggested to be due the fact that for infinite N the CCC-calculated SDCS at any total (excess) energy E should only yield physically meaningful results on the $[0, E/2]$ secondary energy range and zero elsewhere (Bray 1997). In other words, with increasing N the CCC-calculated SDCS should converge to a step-function. Though this is a conceptually useful result, as it allows unambiguous identification of the physical scattering amplitudes, in practice for small-enough E, finite calculations yield oscillatory SDCS and there is small but nonzero flux at secondary energies greater than $E/2$. It is our view that this is a fundamental limitation of the close-coupling approach to ionisation.

Nevertheless, the utility of the approach at low energies is not as diminished as one might at first suspect. The reason why the angular distributions were

relatively unaffected, except by an overall factor obtained from the SDCS, was related to the equivalent-quadrature idea of the pseudostates and an empirical scheme for choosing the states was given (Bray 1999). Consequently, if the true SDCS was available then rescaling all of the angle-differential ionisation cross sections by the ratio of the true to the CCC-calculated SDCS would result in relatively accurate magnitudes also. This idea has been applied successfully to helium, where rescaling factors of approximately two were identified and brought about good agreement with experiment (Bray *et al.* 1998; Rioual *et al.* 1998). This is not so in the case of ionisation of atomic hydrogen by $15{\cdot}6$ eV electrons (Bray 1999), where the estimated rescaling by $2{\cdot}7$ still left the theory a factor of two or so less than experiment.

To complicate things further Bencze and Chandler (1999) have questioned the validity of the CCC approach to ionisation at any energy. They claim that the CCC-calculated ionisation scattering amplitudes as defined by Bray and Fursa (1996*a*) should satisfy the symmetrisation postulate

$$f_S(\boldsymbol{k},\boldsymbol{q}) = (-1)^S f_S(\boldsymbol{q},\boldsymbol{k}) \tag{1}$$

for e–H ionisation, where S is the total spin. The fact that they do not (CCC-calculated SDCS is not symmetric about $E/2$) they take to indicate a lack of convergence everywhere, and presumably, agreement with experiment is coincidental.

Another criticism of our work relates to the incoherent combination of CCC-calculated amplitudes on either side of $E/2$. Whereas this choice was taken in order to retain the unitarity of the close-coupling formalism, Stelbovics (1999) showed that this was not necessary. By studying the S-wave model he showed that the CCC-calculated ionisation amplitude was able to be clearly defined only for $k = q$ and the cross section should be given by

$$\frac{d^3\sigma_S}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{kq}{k_i} \left| f_S^{(N)}(\boldsymbol{k},\boldsymbol{q}) + (-1)^S f_S^{(N)}(\boldsymbol{q},\boldsymbol{k}) \right|^2 , \tag{2}$$

as opposed to the prescription given by Bray and Fursa (1996*a*)

$$\frac{d^3\sigma_S}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{kq}{k_i} \left(|f_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2 + |f_S^{(N)}(\boldsymbol{q},\boldsymbol{k})|^2 \right) , \tag{3}$$

where the $f_S^{(N)}$ are the amplitudes calculated in the CCC theory. Stelbovics (1999) also concluded that the apparent convergence of the CCC results at $E/2$ was real and that it was to half the true scattering amplitude, or one quarter the true cross section. The consequence of his work is profound. It suggests that the CCC method is ideal for equal-energy-sharing kinematics where it is able to yield convergent cross sections in both shape and magnitude fully ab initio without any reference to rescaling.

To address these issues we perform a systematic study of e–H ionisation from high energies through to low. We give our best estimates for the total through to fully differential ionisation cross sections and discuss the issues involved.

2. Theory

The details of the CCC theory have already been given (Bray and Fursa 1996*a*). Here we outline some of the major issues of interest. We begin with the standard Born approximation because it is accurate at high energies and the objections raised by Bencze and Chandler (1999) are equally applicable to our interpretation of this approximation. Unless specified otherwise atomic units are assumed throughout.

(2a) The Born Approximation

If one needs a quick approximate estimate of an excitation scattering process then the Born approximation is an excellent candidate as it covers an immense energy range. The total Hamiltonian H is partitioned asymmetrically as $H = K + V$, where $K = K_1 + H_2$ is the asymptotic Hamiltonian, and where K_1 is the free projectile kinetic energy operator and $H_2 = K_2 + V_2$ is the hydrogen target Hamiltonian. The projectile (target) potential is V_1 (V_2), and $V = V_1 + V_{12}$ is the asymptotic potential, where V_{12} is the electron–electron potential.

The differential cross section for excitation of the hydrogen ground state ϕ_i to state ϕ_f by an electron of incident momentum $\boldsymbol{k}_i$ is approximated via

$$\frac{d\sigma_{fi}}{d\Omega} \approx (2\pi)^4 \frac{k_f}{k_i} |\langle \boldsymbol{k}_f(1)\phi_f(2)|V|\phi_i(2)\boldsymbol{k}_i(1)\rangle|^2 , \tag{4}$$

where the channel states satisfy

$$K|\phi_n(2)\boldsymbol{k}_n(1)\rangle = (\epsilon_n + k_n^2/2)|\phi_n(2)\boldsymbol{k}_n(1)\rangle . \tag{5}$$

In the Born approximation the total wavefunction is simply written as

$$|\Psi_{Si}^{(+)}\rangle \approx |\phi_i \boldsymbol{k}_i\rangle , \tag{6}$$

which neglects antisymmetry (has no dependence on total spin S) or coupling to other channels.

The Born approximation may also be readily applied to ionising collisions, for a total energy $E = \epsilon_i + k_i^2/2 > 0$, by simply replacing the discrete eigenstate ϕ_f in (4) with a continuum eigenstate $\boldsymbol{q}_f^{(-)}$, a Coulomb wave of momentum $\boldsymbol{q}_f$ and energy $q_f^2/2 = E - k_f^2/2$. Then the triply (fully) differential cross section (TDCS) may be written as

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_2} \approx (2\pi)^4 \frac{k_f q_f}{k_i} |\langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)}|V|\phi_i \boldsymbol{k}_i\rangle|^2 . \tag{7}$$

Immediately we run into a problem. In the case of ionisation we have two electrons going out with momenta $\boldsymbol{k}_f$ and $\boldsymbol{q}_f$, typically one much faster than the other. Which one do we assign to the plane wave (electron one) and which to the Coulomb wave (electron two)? Numerical investigation shows that the slower electron should be treated as a Coulomb wave and the faster as a plane wave. This corresponds to a small momentum transfer. However, what do we

do with the Born approximation (7) where $q_f > k_f$? We shall not ignore such terms but rather refer to them as 'double-counting' terms, and write

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_2} \approx (2\pi)^4 \frac{k_f q_f}{k_i} \left(|\langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | V | \phi_i \boldsymbol{k}_i \rangle|^2 + |\langle \boldsymbol{q}_{f'} \boldsymbol{k}_{f'}^{(-)} | V | \phi_i \boldsymbol{k}_i \rangle|^2 \right) , \quad (8)$$

where the plane wave $\langle \boldsymbol{q}_{f'}|$ has momentum $\boldsymbol{q}_{f'} = \boldsymbol{q}_f$ and Coulomb wave $\langle \boldsymbol{k}_{f'}^{(-)}|$ has momentum $\boldsymbol{k}_{f'} = \boldsymbol{k}_f$. The use of the f' index is not necessary here, but we introduce it for later compatibility with the close-coupling approach indicating that the two terms come from different final channels. Interchange of momenta here has nothing to do with exchange. If we were to introduce (Pauli) exchange in (7) we would interchange the coordinate spaces of the plane and Coulomb waves, which is not equivalent to the interchange of momenta in (8).

Without loss of generality let us suppose that $q_f \leq k_f$. For $q_f^2/2 \ll k_f^2/2$ there is no difference between (7) and (8) since the first term in (8) is typically an order of magnitude or more larger than the second. Though the Born approximation works well for such cases, we may wish to apply it at low energies to say demonstrate the difference between the Born approximation and a more realistic theory. In this case the two terms may be of similar magnitude, and we feel that (8) is a more consistent interpretation of the Born approximation utilising solely the rules of non-stationary quantum mechanics.

The primary advantage of the formulation (8) is that the problem of 'double-counting' within the Born approximation (7) is brought out into the open. For example, how should the total ionisation cross section be defined following the definition (7)? Should the endpoint of the energy integration (dE_2) be $E/2$ or E? This question is worthwhile addressing even if in practice the energy integral typically converges well before $E/2$. From our perspective, for the Born approximation (7) (no antisymmetry, electrons are distinguishable) the endpoint of the integration to form the total ionisation cross section σ_I should be E, i.e.

$$\begin{aligned}
\sigma_I &\approx (2\pi)^4 \frac{k_f q_f}{k_i} \int_0^E dE_2 \int d\Omega_1 d\Omega_2 |\langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | V | \phi_i \boldsymbol{k}_i \rangle|^2 \\
&\equiv \int_0^E dE_2 \frac{d\sigma}{dE_2}(E_2) \qquad (9) \\
&= \int_0^{E/2} dE_2 \left[\frac{d\sigma}{dE_2}(E_2) + \frac{d\sigma}{dE_2}(E - E_2) \right] \qquad (10) \\
&\equiv (2\pi)^4 \frac{k_f q_f}{k_i} \int_0^{E/2} dE_2 \int d\Omega_1 d\Omega_2 \left(|\langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | V | \phi_i \boldsymbol{k}_i \rangle|^2 \right. \\
&\quad \left. + |\langle \boldsymbol{q}_{f'} \boldsymbol{k}_{f'}^{(-)} | V | \phi_i \boldsymbol{k}_i \rangle|^2 \right) , \qquad (11)
\end{aligned}$$

where $E_2 = q_f^2/2$. Thus, as far as the Born approximation to e–H ionisation is concerned, as the difference in the energies of the two outgoing electrons increases one term in (8) and (11) converges to the true scattering amplitude, whereas the

other converges to zero. The inherent 'double-counting' problem is clear to see, and occurs in the close-coupling formalism in an exactly the same way.

The objections of Bencze and Chandler (1999) are applicable to our interpretation of the Born approximation. The symmetrisation postulate (1) is not satisfied as there is no spin-dependence. Nevertheless, the Born approximation has value over an immense kinematical range.

(2b) The Close-coupling with No Exchange Approximation

To improve on the Born approximation we need to allow for coupling to other channels and antisymmetry of the total wave function. We consider the former first. Improvement on (6) is provided by the approximation

$$\begin{aligned} |\Psi_{Si}^{(+)}\rangle \approx |\Psi_i^{(+)}\rangle &\approx I_2^{(N)}|\Psi_i^{(+)}\rangle \\ &= \sum_{n=1}^{N} |\phi_n^{(N)}\rangle\langle\phi_n^{(N)}|\Psi_i^{(+)}\rangle \\ &= \sum_{n=1}^{N} |\phi_n^{(N)} f_{ni}^{(N+)}\rangle\,, \end{aligned} \tag{12}$$

where the N functions $\phi_n^{(N)}$ form an orthonormal set, and the functions $f_{ni}^{(N+)}$ we obtain by solving the spin-independent close-coupling equations for the T matrix:

$$\begin{aligned} \langle \boldsymbol{k}_f \phi_f^{(N)}|T|\phi_i^{(N)}\boldsymbol{k}_i\rangle &\equiv \langle \boldsymbol{k}_f \phi_f^{(N)}|V|\sum_{n=1}^{N}\phi_n^{(N)} f_{ni}^{(N+)}\rangle \\ &= \langle \boldsymbol{k}_f \phi_f^{(N)}|V|\phi_i^{(N)}\boldsymbol{k}_i\rangle \\ &\quad + \sum_{n=1}^{N}\int d^3k\, \frac{\langle \boldsymbol{k}_f \phi_f^{(N)}|V|\phi_n^{(N)}\boldsymbol{k}\rangle\langle \boldsymbol{k}\phi_n^{(N)}|T|\phi_i^{(N)}\boldsymbol{k}_i\rangle}{E+i0-\epsilon_n^{(N)}-k^2/2}\,. \end{aligned} \tag{13}$$

The expansion states $\phi_n^{(N)}$ must be square-integrable in order that all of the V-matrix elements are calculable. Furthermore, we desire that

$$\lim_{N\to\infty} I_2^{(N)}|\Psi_i^{(+)}\rangle = I_2|\Psi_i^{(+)}\rangle = |\Psi_i^{(+)}\rangle\,, \tag{14}$$

where I_2 is the true target-space identity operator. This may be achieved by diagonalising the target Hamiltonian $H_2 = K_2 + V_2$ using a Laguerre basis to yield $\phi_n^{(N)}$ such that

$$\langle \phi_f^{(N)}|H_2|\phi_i^{(N)}\rangle = \delta_{fi}\epsilon_f^{(N)}\,. \tag{15}$$

The diagonalisation (15) results in states with negative and positive energies. With increasing N the negative energy states $\phi_f^{(N)} \to \phi_f$, the true discrete eigenstates, and the positive energy states provide an increasingly dense discretisation of the continuum.

The close-coupling approximation (without exchange) builds on top of the Born approximation and so has the same asymptotic Hamiltonian and channel functions. It is unitary and the sum over n implies an on-shell integration over the continuum from zero to total energy E. The transition matrix is

$$\langle \boldsymbol{k}_f \phi_f | T | \phi_i \boldsymbol{k}_i \rangle \equiv \langle \boldsymbol{k}_f \phi_f | V | \Psi_{Si}^{(+)} \rangle \approx \langle \boldsymbol{k}_f \phi_f | I_2^{(N)} V I_2^{(N)} | \Psi_i^{(+)} \rangle$$
$$\approx \langle \phi_f | \phi_f^{(N)} \rangle \langle \boldsymbol{k}_f \phi_f^{(N)} | T | \phi_i^{(N)} \boldsymbol{k}_i \rangle \,, \qquad (16)$$

where the N-state T matrix is obtained from (13), and the states $\phi_n^{(N)}$ have been obtained in such a way that given a particular eigenstate ϕ_f of energy ϵ_f (discrete or continuous), for some $n = f$ we have $\epsilon_f^{(N)} = \epsilon_f$, and hence

$$\langle \phi_f | \phi_n^{(N)} \rangle \approx \delta_{fn} \langle \phi_f | \phi_f^{(N)} \rangle \,. \qquad (17)$$

For discrete $\epsilon_f < 0$ we need N to be sufficiently large so that $\langle \phi_f | \phi_f^{(N)} \rangle \approx 1$ and $\langle \phi_i | \phi_i^{(N)} \rangle \approx 1$. In this case we use the T matrix calculated in (13) directly. For $\epsilon_f > 0$ with $\langle \phi_f | \equiv \langle \boldsymbol{q}_f^{(-)} |$ the T matrix in (13) is multiplied by the overlap $\langle \boldsymbol{q}_f^{(-)} | \phi_f^{(N)} \rangle$, which has the effect of restoring the continuum boundary conditions and introduces a one-electron Coulomb phase.

The close-coupling without exchange N-state approximation to the experimentally measured TDCS is

$$\frac{d^3\sigma^{(N)}}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{k_f q_f}{k_i} \Big(|\langle \boldsymbol{q}_f^{(-)} | \phi_f^{(N)} \rangle \langle \boldsymbol{k}_f \phi_f^{(N)} | T | \phi_i^{(N)} \boldsymbol{k}_i \rangle|^2$$
$$+ |\langle \boldsymbol{k}_{f'}^{(-)} | \phi_{f'}^{(N)} \rangle \langle \boldsymbol{q}_{f'} \phi_{f'}^{(N)} | T | \phi_i^{(N)} \boldsymbol{k}_i \rangle|^2 \Big) \,. \qquad (18)$$

This is a generalisation of (8), with the f' notation clearly indicating that the two terms come from very different final channels. With such a definition the SDCS is symmetric about $E/2$ and the total ionisation cross section would be obtained by integration to $E/2$. It is helpful to think of the second term in (13) as a second order correction to the Born approximation. As such, it vanishes at high energies leaving just the Born approximation for both the discrete excitation and ionising collisions. Numerically, we find

$$\langle \boldsymbol{q}_f^{(-)} | \phi_f^{(N)} \rangle \langle \boldsymbol{k}_f \phi_f^{(N)} | V | \phi_i^{(N)} \boldsymbol{k}_i \rangle \approx \langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | V | \phi_i^{(N)} \boldsymbol{k}_i \rangle$$

to a high accuracy due to the short-ranged $\phi_i^{(N)}$ negating the long-range behaviour of $\boldsymbol{q}_f^{(-)}$.

For unequal energy-sharing the two terms in (18) are very different and converge to their respective Born approximations with increasing energy. In this case the first term converges to the true scattering amplitude while the second converges to zero.

Note that for equal energy-sharing $f = f'$, but the two terms are still generally different owing to the vector nature of momenta. They are equal to each other for the so-called coplanar doubly symmetric ($E_A = E_B$ and $\theta_A = -\theta_B$) geometry.

However, while exchange is neglected this approximation will not work well for this special case, and has only value whenever the SDCS at $E/2$ is very much smaller than for the highly asymmetric energy-sharing.

Like the Born approximation, the close-coupling with no exchange approximation appears to have a double-counting problem. There are two independent estimates in (18) of a single ionisation process.

(2c) The Close-coupling with Exchange Approximation

In the momentum-space formulated close-coupling equations (13), introduction of exchange results in a simple modification of the interaction potential V by $V_S = V + (-1)^S(H-E)P_r$, where P_r is the space exchange operator (Bray and Stelbovics 1992). We then solve

$$\langle \boldsymbol{k}_f \phi_f^{(N)} | T_S | \phi_i^{(N)} \boldsymbol{k}_i \rangle = \langle \boldsymbol{k}_f \phi_f^{(N)} | V_S | \phi_i^{(N)} \boldsymbol{k}_i \rangle + \sum_{n=1}^{N} \int d^3k \, \frac{\langle \boldsymbol{k}_f \phi_f^{(N)} | V_S | \phi_n^{(N)} \boldsymbol{k} \rangle \langle \boldsymbol{k} \phi_n^{(N)} | T_S | \phi_i^{(N)} \boldsymbol{k}_i \rangle}{E + i0 - \epsilon_n^{(N)} - k^2/2} \tag{19}$$

separately for $S = 0, 1$. Subsequently, the S-dependent differential cross sections are obtained using (18), i.e.

$$\frac{d^3\sigma_S^{(N)}}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{k_f q_f}{k_i} \left(|\langle \boldsymbol{q}_f^{(-)} | \phi_f^{(N)} \rangle \langle \boldsymbol{k}_f \phi_f^{(N)} | T_S | \phi_i^{(N)} \boldsymbol{k}_i \rangle|^2 + |\langle \boldsymbol{k}_{f'}^{(-)} | \phi_{f'}^{(N)} \rangle \langle \boldsymbol{q}_{f'} \phi_{f'}^{(N)} | T_S | \phi_i^{(N)} \boldsymbol{k}_i \rangle|^2 \right) , \tag{20}$$

and the CCC-calculated spin-averaged cross section for e–H ionisation is evaluated as

$$\frac{d^3\sigma^{(N)}}{d\Omega_1 d\Omega_2 dE_2} = \tfrac{1}{4} \frac{d^3\sigma_0^{(N)}}{d\Omega_1 d\Omega_2 dE_2} + \tfrac{3}{4} \frac{d^3\sigma_1^{(N)}}{d\Omega_1 d\Omega_2 dE_2} . \tag{21}$$

The close-coupling with exchange approximation is equivalent to

$$|\Psi_{Si}^{(+)}\rangle \approx (1 + (-1)^S P_r) \sum_{n=1}^{N} |\phi_n^{(N)} f_{Sni}^{(N+)}\rangle . \tag{22}$$

Thus, the total wave function is antisymmetric in all space of the two electrons, but is zero when both r_1 and r_2 are large.

The change from V to V_S is not entirely trivial. There are extra computational difficulties due to non-uniqueness problems, but these have been dealt with adequately; see Bray and Stelbovics (1992) for details.

With increasing total energy E the contribution of the exchange part of V_S diminishes faster than the direct part V. Eventually we may totally drop exchange to obtain (13), and with further increase of energy obtain the Born approximation.

Introducing exchange to the close-coupling formalism does not result in the scattering amplitudes obeying the symmetrisation postulate (1). In particular, we have

$$\langle \boldsymbol{q}_f^{(-)}|\phi_f^{(N)}\rangle\langle \boldsymbol{k}_f\phi_f^{(N)}|T_S|\phi_i^{(N)}\boldsymbol{k}_i\rangle \neq (-1)^S\langle \boldsymbol{k}_{f'}^{(-)}|\phi_{f'}^{(N)}\rangle\langle \boldsymbol{q}_{f'}\phi_{f'}^{(N)}|T_S|\phi_i^{(N)}\boldsymbol{k}_i\rangle \qquad (23)$$

generally, though we shall see that for $q_f = k_f$ near equality does hold. Note that though $\boldsymbol{q}_{f'} = \boldsymbol{q}_f$ and $\boldsymbol{k}_{f'} = \boldsymbol{k}_f$ the two states $\phi_f^{(N)}$ and $\phi_{f'}^{(N)}$ are very different for $f \neq f'$. Bencze and Chandler (1999) claim [equation (20) of their paper says that the CCC amplitudes converge to the true amplitudes] that in the limit of infinite N there should be equality in (23), and hence double counting of the ionisation cross sections. While we are unable to perform such calculations, the fact that the two terms converge to their respective Born estimates with increasing energy indicates that their derivation is in error. The source of the error we suspect to be in the way the limit $N \to \infty$ is taken, ignoring how this affects the close-coupling boundary conditions. What we do observe, with increasing N, is that the close-coupling with exchange calculations yield diminishing cross sections for amplitudes $\langle \boldsymbol{q}_{f'}\phi_{f'}^{(N)}|T_S|\phi_i^{(N)}\boldsymbol{k}_i\rangle$, where $q_{f'}^2/2 < \epsilon_{f'}^{(N)}$. This has led to the suggestion that the CCC calculations should converge to a step-function SDCS (Bray 1997), with numerical problems arising whenever the size of the step at $E/2$ is substantial. This idea has gained further support from Miyashita *et al.* (1999) and Baertschy *et al.* (1999) who studied the e–H S-wave model. Unfortunately, a mathematical proof is still lacking, though the recent work of Stelbovics (1999), described below, has gone very close to doing so.

Introduction of exchange removes the distinguishability between the two electrons of energy $\epsilon_f^{(N)}$ and $E - \epsilon_f^{(N)}$ for a particular ionisation process, however, this process is still calculated twice: once with the electron of energy $\epsilon_f^{(N)}$ being treated by a pseudostate and once as a plane wave. It is these two treatments of a single ionisation process that imply double-counting, even in a unitary theory. The step-function idea says that for infinite N one of these is zero.

(2d) Equal Energy-sharing Kinematics

Most recently Stelbovics (1999) has made substantial progress in the understanding of the problem. By also studying the S-wave model within the true eigenstate close-coupling formalism he deduced that the unitarity relation is satisfied with the secondary energy integration ending at $E/2$. This implies a step function behaviour of the underlying ionisation amplitudes which may be defined for all $0 < q_f^2/2 < E$. In other words, $\langle \boldsymbol{k}_f\boldsymbol{q}_f^{(-)}|T_S|\phi_i\boldsymbol{k}_i\rangle$ are zero for $q_f > k_f$. This is a very important result, even though no numerical method has yet been devised for solving close-coupling equations with true discrete and continuous eigenstates, because the formalism of the CCC method is such that for infinite N the expansion over the pseudostates is equivalent to the expansion over the eigenstates. Hence, if the latter yields step-function ionisation amplitudes then so should the former.

Stelbovics (1999) also considered how to define the ionisation amplitudes compatible with formal ionisation theory following a CCC-type calculation. Note that our above discussion suggested a way of defining the cross sections, not

the underlying amplitudes which is not possible due to the double-counting problem. He independently concluded also that in general it is impossible to define the ionisation amplitudes unambiguously, unless the amplitudes exhibit the step-function behaviour. However, he showed that at equal-energy-sharing the true ionisation amplitudes $f_S(\boldsymbol{k},\boldsymbol{q})$ may always be deduced from those obtained in the CCC theory,

$$f_S^{(N)}(\boldsymbol{k}_f,\boldsymbol{q}_f) = \langle \boldsymbol{q}_f^{(-)}|\phi_f^{(N)}\rangle\langle \boldsymbol{k}_f\phi_f^{(N)}|T_S|\phi_i^{(N)}\boldsymbol{k}_i\rangle\,, \tag{24}$$

by

$$f_S(\boldsymbol{k},\boldsymbol{q}) = f_S^{(N)}(\boldsymbol{k},\boldsymbol{q}) + (-1)^S f_S^{(N)}(\boldsymbol{q},\boldsymbol{k})\,. \tag{25}$$

Consequently, he concluded that the CCC-calculated $k = q$ amplitudes did converge with increasing N, but to half the true scattering amplitude, at least in the model considered. The cross sections are obtained from $|f_S(\boldsymbol{k},\boldsymbol{q})|^2$, as opposed to the integral preserving estimate we suggested $|f_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2 + |f_S^{(N)}(\boldsymbol{q},\boldsymbol{k})|^2$, see equation (20). Can the two prescriptions be reconciled?

Firstly, given the observation of Stelbovics (1999) that the CCC amplitudes converge to half the true amplitudes for the model problem, we suppose this is also the case for the full problem and so our prescription yields cross sections a factor of 2 too low in all equal-energy-sharing cases. This has been previously observed in the case of e–He ionisation at 64·6 eV (Bray *et al.* 1997), 44·6 eV (Rioual *et al.* 1998) and 32·6 eV (Bray *et al.* 1998). Thus, only for equal-energy-sharing should we have an extra factor of 2 multiplying the incoherent combination of the $f_S^{(N)}$. Being only at a single point this does not affect the integral that leads to the correct total ionisation cross section.

Now, we have noted earlier (Bray *et al.* 1997) that the two terms $|f_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2$ and $|f_S^{(N)}(\boldsymbol{q},\boldsymbol{k})|^2$ are visibly different and are necessary together to yield accurate angular distributions. If we write

$$f_S^{(N)}(\boldsymbol{k},\boldsymbol{q}) = (-1)^S f_S^{(N)}(\boldsymbol{q},\boldsymbol{k}) + \delta_S^{(N)}(\boldsymbol{k},\boldsymbol{q})\,, \tag{26}$$

where $\delta_S^{(N)}$ is some (small) number, then

$$2(|f_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2 + |f_S^{(N)}(\boldsymbol{q},\boldsymbol{k})|^2) = |f_S^{(N)}(\boldsymbol{k},\boldsymbol{q}) + (-1)^S f_S^{(N)}(\boldsymbol{q},\boldsymbol{k})|^2 + |\delta_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2\,. \tag{27}$$

On the other hand, the difference between $|f_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2$ and $|f_S^{(N)}(\boldsymbol{k},\boldsymbol{q}) - \delta_S^{(N)}(\boldsymbol{k},\boldsymbol{q})|^2$ may be much more substantial.

Thus, the coherent and incoherent combinations of amplitudes in (27) are effectively simply doublings. The claim (26) (assuming small $\delta_S^{(N)}$) is a very strong one. For it to be satisfied the calculated matrix elements must satisfy some special properties. Consider the CCC-calculated amplitude in partial wave form

$$f_{JS}^{(N)}(Lk,lq) = e^{i\sigma_l(q)}|\langle q_l^{(-)}|\phi_{fl}^{(N)}\rangle|\langle k_L\phi_{fl}^{(N)}|T_{JS}|\phi_{i0}^{(N)}k_0\rangle\,, \tag{28}$$

where J is the total orbital angular momentum, $\epsilon_{fl}^{(N)} = q^2/2$ and $\sigma_l(q)$ is the full complex phase arising from the overlap $\langle q_l^{(-)}|\phi_{fl}^{(N)}\rangle$. Given that $k = q$, interchange of l and L has the effect of explicitly changing the phase as well as the T-matrix obtained from (19). Yet together, the resulting amplitudes satisfy the partial-wave expanded (26). Furthermore, since $l \leq l_{\max}$ with $|J - l| \leq L \leq J + l$, we need sufficiently large $l_{\max}$ that interchange of L and l was possible for all substantial T_{JS}. To demonstrate (27) graphically, in all of the following figures that present equal-energy-sharing kinematics we give both sides of (27) for the two spins.

One may ask which of the two sides of (27) is more accurate. Unfortunately, even equality does not guarantee accuracy of the amplitudes, only correct symmetry. In other words, satisfaction of (27) is necessary, but not sufficient. The right side of (27) has the advantage of looking compatible with an indistinguishable treatment of the two electrons, and so being able to readily define the final amplitude to be used in generating the cross sections, which will always have the correct symmetry irrespective of what the underlying CCC amplitude is. This is a strength and a weakness, as it looses sensitivity to the accuracy of the CCC calculation. The left side of (27) is more sensitive, since for example, for the doubly symmetric geometry both terms must yield zero for the triplet case. The right side has the advantage of not requiring the step-function idea or the combination of amplitudes at $E/2$ as a limiting procedure of amplitudes on either side of $E/2$. The most sensitive test would be to simply use $2f_S^{(N)}(\boldsymbol{k}, \boldsymbol{q})$ or $2f_S^{(N)}(\boldsymbol{q}, \boldsymbol{k})$ as the amplitudes. The factor of 2 is due to the convergence to half the true magnitude at $E/2$.

We should mention that the demonstration of failure of a coherent combination of amplitudes for e–He equal-energy-sharing ionisation at 64·6 eV (Bray *et al.* 1997) was due to the fact that in the case of helium the correct coherent combination is more complicated, and requires derivation along the lines given by Stelbovics (1999) for the e–H system. The one given,

$$\sum_{s=0,1} |F_s^{(N)}(\boldsymbol{k}, \boldsymbol{q}) + F_s^{(N)}(\boldsymbol{q}, \boldsymbol{k})|^2 \,,$$

where s is the spin of the frozen-core two-electron continuum wave, yields the wrong answer. The intuitive combination

$$|F_0^{(N)}(\boldsymbol{k}, \boldsymbol{q}) + F_1^{(N)}(\boldsymbol{q}, \boldsymbol{k})|^2 + |F_1^{(N)}(\boldsymbol{k}, \boldsymbol{q}) + F_0^{(N)}(\boldsymbol{q}, \boldsymbol{k})|^2$$

yields a factor of 2 difference from the incoherent combination used, but requires formal derivation.

(2e) Asymmetric Energy-sharing Kinematics

What about asymmetric energy-sharing? Stelbovics (1999) shows that different logarithmic phases on either side of $E/2$ lead to difficulty in defining the ionisation amplitudes, unless the CCC-calculated amplitude for $q > k$ is identically zero. Though we are as yet unable to prove analytically the step-function hypothesis, which Bencze and Chandler (1999) believe to have proved to be incorrect, all of our numerical evidence is consistent with it. Certainly, for the purpose of

making comparison with experiment, it holds in our finite calculations for the substantially asymmetric excess energy-sharing kinematics. In these cases the second term in (20) is insignificant compared to the first. Does the first term yield the true scattering amplitude? When convergent, as it is at high energies (Bray and Fursa 1996*a*), we suspect so. This is also implied by the analysis of Stelbovics (1999). At sufficiently low energies we find that convergence to a desirable accuracy is unable to be obtained for the SDCS with $q < k$. Our choices are then to present results as they are, or attempt to estimate what the true SDCS should be and rescale the CCC-calculated TDCS to this SDCS.

How can we estimate what the true SDCS might be? Fortunately, the underlying physics suggests that the functional form of the SDCS is likely to be simple and, at sufficiently low energies, may be modelled relatively accurately by a quadratic. We already know the integral accurately ab initio and the point of symmetry, requiring just one more parameter to fix the quadratic. To do so Bray *et al.* (1998) have observed that the value of the e–He SDCS at zero secondary energy was quite stable and used this to fix the estimate of the true SDCS. The resultant rescaling leads to an increase by factor of approximately 2 in the CCC-calculated TDCS at equal-energy-sharing, and good agreement with absolute experiment. A similar idea was used for the e–H system at $15{\cdot}6$ eV (Bray 1999), resulting in an increase by a factor of $2{\cdot}7$, still a further factor of 2 below the experimental absolute value determination.

The oscillations in the CCC-calculated SDCS have been well-documented, and we have been unable to explain, until now, the apparent convergence of the CCC results at equal-energy-sharing (Bray 1997, 1999; Bray *et al.* 1997; Röder *et al.* 1997*a*; Rioual *et al.* 1998). Now, thanks to the analysis of Stelbovics (1999), we know the value of the true SDCS at $E/2$. This SDCS, calculated according to (9) or (10), is a factor of 4 or 2 lower than the true SDCS, respectively. This has been tested by comparison with the benchmark SDCS calculations of Baertschy *et al.* (1999) as reported by Stelbovics (1999).

Another strong test of this idea is found by consideration of double photoionisation (DPI). Here the CCC method has yielded accurate total (Kheifets and Bray 1998*b*) and differential (Kheifets and Bray 1998*a*; Braeuning *et al.* 1998) ionisation cross sections. The rescaling of the CCC TDCS relied on the work of Pont and Shakeshaft (1995) who gave demonstrably accurate estimates of the total cross sections, and arguably equally accurate estimates of the SDCS($E/2$), from 2 to 80 eV above threshold. This is particularly helpful for us as it allows a thorough comparison of the CCC-calculated SDCS($E/2$). We have performed this check for the published CCC-calculated DPI SDCS, and at the excess energies presented here, and find generally approximately a factor of 2 difference, as expected.

Accordingly, rather than assuming a stable SDCS(0) derived from examination of near threshold total ionisation cross sections, we fix the third parameter of the quadratic estimate of the SDCS by the estimate of the true SDCS($E/2$) obtained from the raw CCC-calculated SDCS($E/2$) multiplied by 4, i.e. the same value as obtained from either side of (27). This is particularly helpful in the present e–H ionisation case, where the close-coupling equations are solved separately for the two total spins. For each total spin, rather than attempting to estimate SDCS(0), we simply obtain SDCS($E/2$) directly from the CCC calculations, and hence the quadratic SDCS estimate.

3. Results and Discussion

Before looking at the detailed results of the individual energies considered, we present in Fig. 1 the total ionisation cross section (TICS) and its spin asymmetry as a function of energy. The CCC calculations at the individual energies (solid dots) will be detailed later. We see excellent agreement between the CCC calculations and the experiment, with the exception of the data of Shyn (1992). The experimental technique of Shah *et al.* (1987) is specifically aimed at the total ionisation cross section, whereas Shyn (1992) obtained it after a double integration of doubly differential cross section (DDCS) measurements. Good agreement with the spin asymmetries indicates correct spin-dependent total ionisation cross sections at all energies. The quality of agreement between theory and experiment was first presented by Bray and Stelbovics (1993). Since that time other close-coupling methods have also obtained similar results (Kato and Watanabe 1995; Bartschat and Bray 1996; Scott *et al.* 1997).

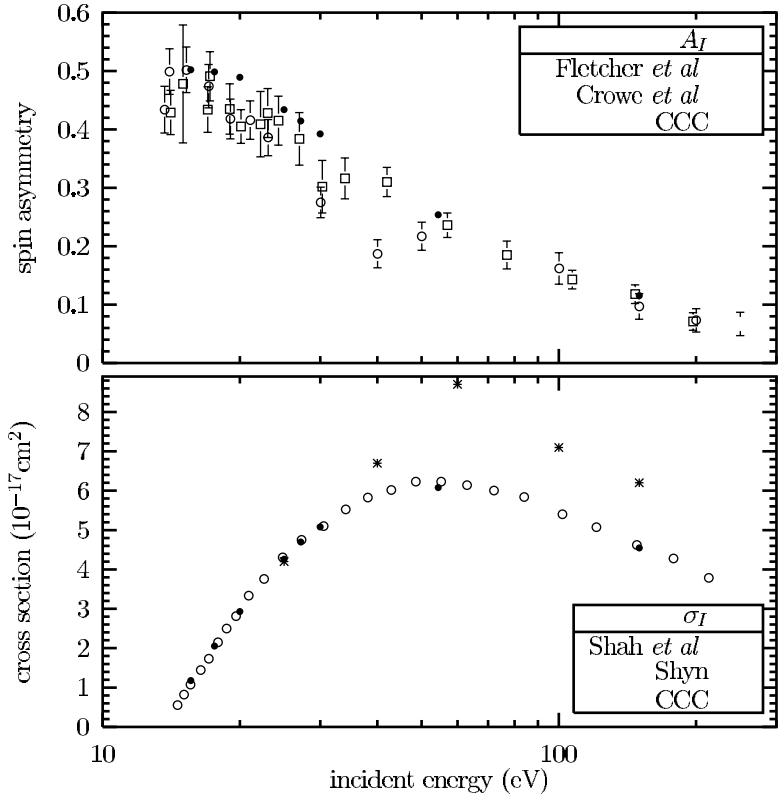

Fig. 1. Total ionisation cross section σ_I and its spin asymmetry A_I as a function of energy. The present results are denoted by CCC and the measurements are due to Shah *et al.* (1987), Crowe *et al.* (1990), Fletcher *et al.* (1985) and Shyn (1992).

The utility of the CCC calculations depends on obtaining convergence with increasing $N = \sum_l N_l$. This means convergence with target-space angular momentum $l_{\max}$ and number of states N_l within each l. We take $N_l = N_0 - l$ as this leads to a similar integration rule in the continuum for each l, of

importance at low energies (Bray 1999). This allows convenient labelling of the calculations by CCC($N_0, l_{\max}$). All of the calculations performed required substantial computational resources. The higher energy calculations required around 1 G of RAM, while the lower energy ones required up to 2 G of RAM.

At high enough energies most theories, those that satisfy the symmetrisation postulate, and those that do not, yield much the same results for highly asymmetric energy-sharing kinematics. We wish to demonstrate that the CCC differential cross sections as defined in (20) and (18) also do so.

(3a) Incident Electron Energy 250 eV

We begin our study with $E_0 = 250$ eV. In performing the calculations we need to be mindful of which experiment we wish to describe. The experiment of Ehrhardt *et al.* (1986) has $E_B = 5$ eV, and so we ensure, by varying the Laguerre exponential fall-off parameter λ_l (Bray and Stelbovics 1992), that one of the states $\phi_{nl}^{(N)}$ had the energy $\epsilon_{nl}^{(N)} = 5$ eV. A number of CCC($N_0, l_{\max}$) calculations were performed, but we present the results from only the largest, CCC(15,5), which couples a total of 75 states.

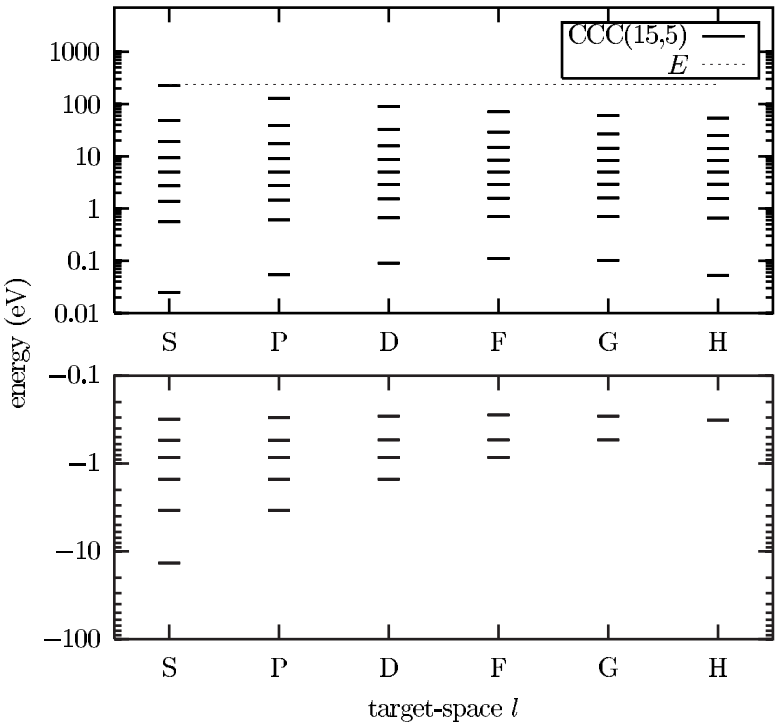

Fig. 2. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 250 eV e–H calculation using the CCC(15,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was 5 eV.

The energy levels of the CCC(15,5) calculation are given in Fig. 2. We see that the choice of states has led to a systematic treatment of both the discrete and the continuous spectrum. Negative-energy states with $n \leq 6$ have arisen. The $n \leq 5$ are good eigenstates, with the $n = 6$ states taking into account all true $n \geq 6$ discrete eigenstates. The positive energies are approximately similarly spaced for

each l, particularly in the region of 5 eV. The total energy $E = 250$–$13{\cdot}6$ eV is greater than all of the state energies, and hence all channels are open. The energy levels increase approximately exponentially, and so the energy region $[0, E/2]$ is much more densely covered than $[E/2, E]$.

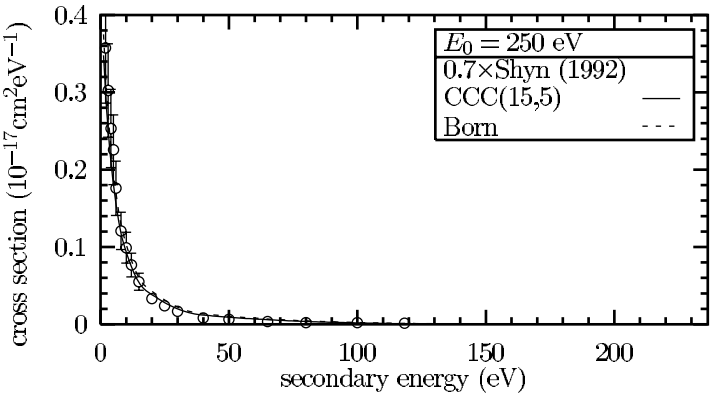

Fig. 3. Singly differential cross section for 250 eV electron-impact ionisation of the ground state of atomic hydrogen. The data of Shyn (1992) have been scaled for consistency with the data of Shah *et al.* (1987), see Fig. 1.

In Fig. 3 we consider the SDCS arising from the CCC(15,5) calculation. This we obtain directly from the integrated cross sections for the excitation of the positive-energy pseudostates (Bray and Fursa 1995), equivalent to (9). Comparison with the data of Shyn (1992) is given after the latter have been reduced by a factor of $0{\cdot}7$. This reduction brings the experimental SDCS into consistency with the data of Shah *et al.* (1987). There is almost no difference between the Born approximation and the CCC(15,5) result. Both yield excellent agreement with the rescaled experiment, though neither are symmetric about $E/2$ and hence do not satisfy the symmetrisation postulate (1). The theoretical SDCS at $E/2$ is practically zero and remains so at higher secondary energies. The true, experimentally measurable SDCS, would be symmetric about $E/2$, but there is no new physics in this and does not invalidate the Born or CCC results for the smaller secondary energies.

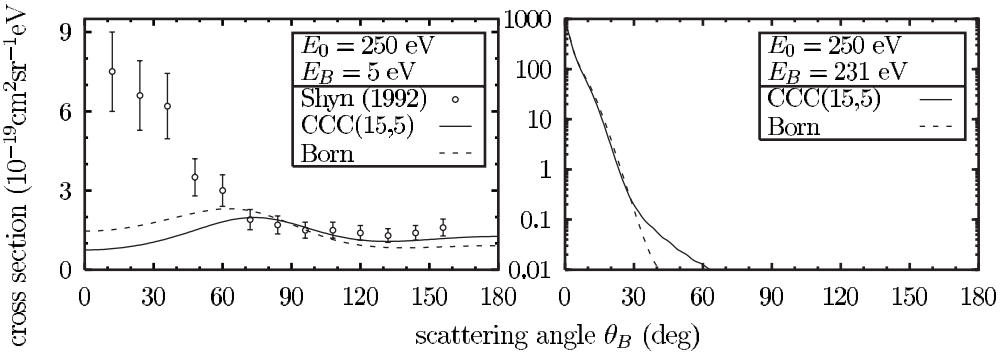

Fig. 4. Doubly differential cross section of the 5 and 231 eV outgoing electrons for 250 eV electron-impact ionisation of the ground state of atomic hydrogen.

The DDCS are given in Fig. 4. Unscaled data are compared with the CCC and Born calculations. We see good agreement at the backward angles suggesting that the experiment had some systematic problem at the lower scattering angles. There is a small difference between the Born and CCC calculations, but generally the two are very similar. We also performed a CCC(15,5) calculation with no exchange. This is indistinguishable from the presented CCC(15,5) one, indicating that the difference with Born is due solely to coupling. The discrepancy with experiment at forward angles is similar to that reported by Berakdar and Klar (1993).

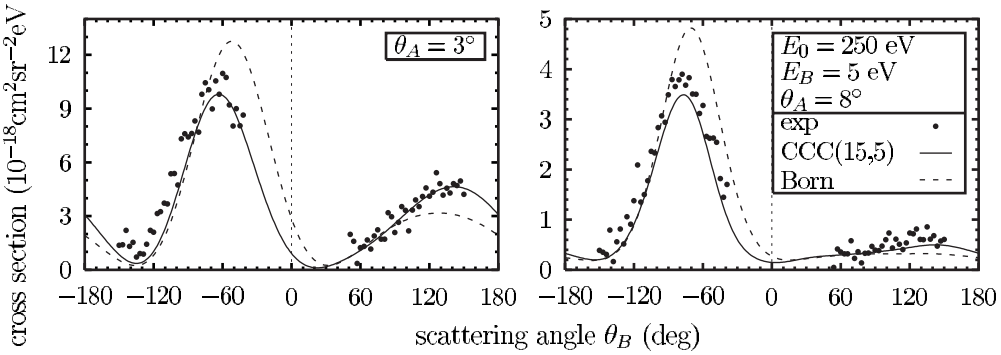

Fig. 5. Coplanar triply differential cross section of the E_B =5 eV electron with the E_A =231 eV electron being detected at specified θ_A scattering angle for 250 eV electron-impact ionisation of the ground state of atomic hydrogen. The absolute measurements are due to Ehrhardt *et al.* (1986). Negative angles correspond to the opposite side of the incident beam to the positive angles.

Lastly, for this incident energy, the TDCS are presented in Fig. 5. We see a small difference between the Born and the CCC calculation, with the latter giving complete agreement with experiment. Comparison with the CCC(15,5) no exchange calculation, which is pictorially indistinguishable from the CCC(15,5) one presented, indicates that the improvement on the Born approximation is again solely due to coupling.

In our view, the results presented at this energy are sufficient to invalidate the arguments of Bencze and Chandler (1999). Here the close-coupling formalism yields results much the same as the Born approximation and experiment. This is not fortuitous. The second term in (20) is essentially zero, with the first term, in our view, having converged to the true ionisation scattering amplitudes of the problem considered.

(3b) Incident Electron Energy 150 eV

We have considered e–H ionisation at 150 eV in the very first application of the CCC method to differential ionisation cross sections (Bray *et al.* 1994). The formalism used then varies a little from the present in that following Curran and Walters (1987) an attempt was previously made to incorporate the treatment of higher target-space orbital angular momentum than the $l_{\max}$ used within the close-coupling equations. We no longer do so, believing that it is more consistent to extract all of the ionisation information from only the matrix elements arising upon the solution of the close-coupling equations.

At this energy we have absolute experimental TDCS for three secondary energies $E_B = 3$, 5 and 10 eV (Ehrhardt *et al.* 1986). In a single calculation we may vary λ_l to obtain only one of the E_B. The TDCS at other E_B have to be obtained with the assistance of interpolation (Bray and Fursa 1996*a*). Three CCC(15,5) calculations were performed with λ_l varied to obtain each of the three E_B. Comparison of the full set of TDCS showed little variation and so we

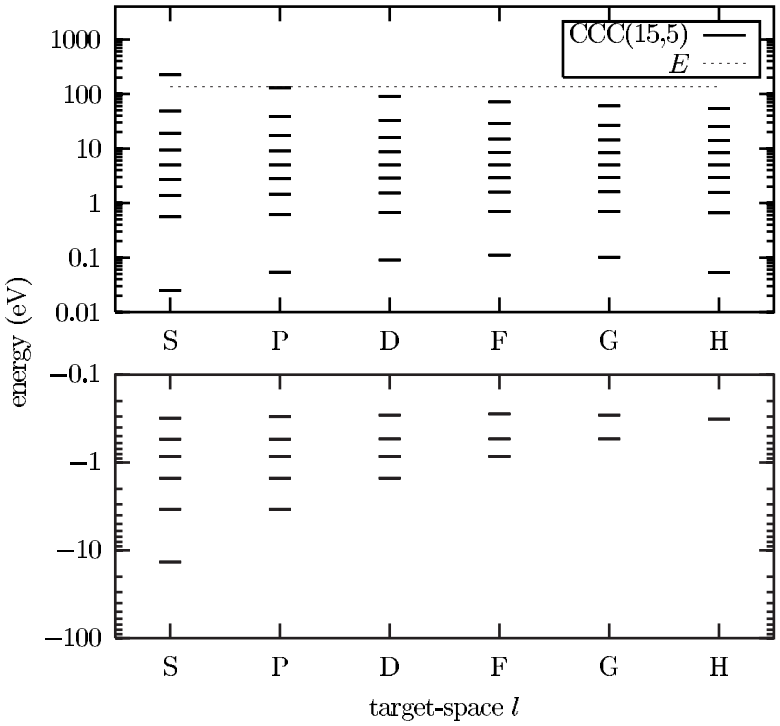

Fig. 6. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 150 eV e–H calculation using the CCC(15,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was 5 eV.

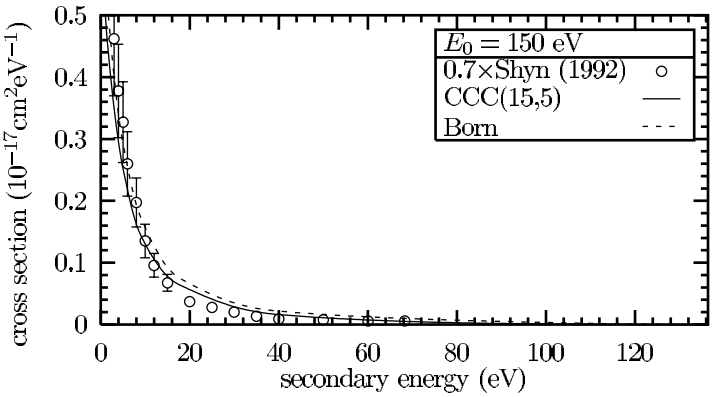

Fig. 7. Singly differential cross section for 150 eV electron-impact ionisation of the ground state of atomic hydrogen. The data of Shyn (1992) have been scaled for consistency with the data of Shah *et al.* (1987), see Fig. 1.

present the results just from the calculation where the λ_l were varied to obtain $E_B = 5$ eV. The energy levels of this CCC(15,5) calculation are given in Fig. 6. We see that the choice of states is very similar to the case of 250 eV incident energy (Fig. 2). The total energy $E = 150\text{–}13{\cdot}6$ eV is greater than all but one of the state energies.

In Fig. 7 the SDCS arising from the calculation is considered. Comparison with the data of Shyn (1992) is given after the latter have been reduced by again a factor of $0{\cdot}7$. There is now some visible difference between the Born approximation and the CCC(15,5) result. Again, no exchange calculations show that this is due to neglect of coupling in the Born approximation. Both yield good agreement with the rescaled experiment. The SDCS($E/2$) is practically zero and hence, we suspect, there are no convergence problems.

The DDCS are given in Fig. 8. Unscaled data of Shyn (1992) are compared with the CCC and Born calculations. As one might expect the difference between Born and CCC is somewhat bigger at this energy than at 250 eV. The smaller visible difference in the SDCS is due to the 'crossing-over' of the two curves. The agreement with experiment is only acceptable at intermediate and backward

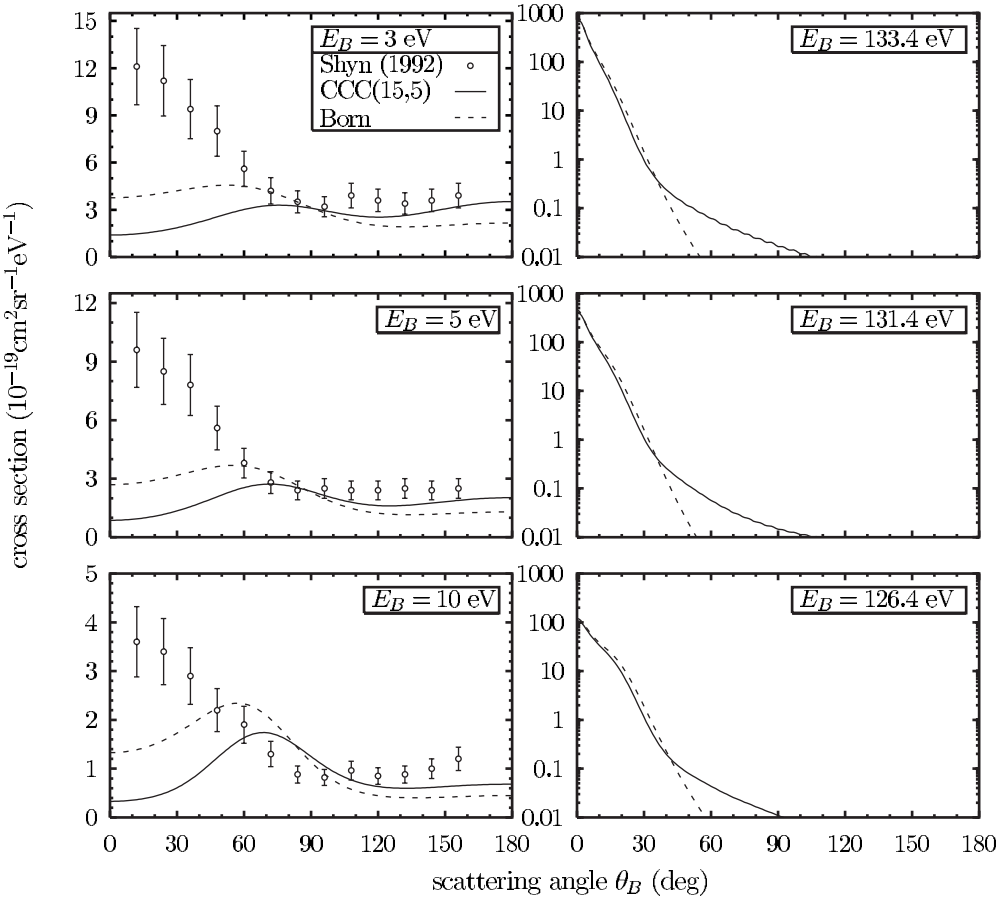

Fig. 8. Doubly differential cross section of the indicated outgoing electrons for 150 eV electron-impact ionisation of the ground state of atomic hydrogen.

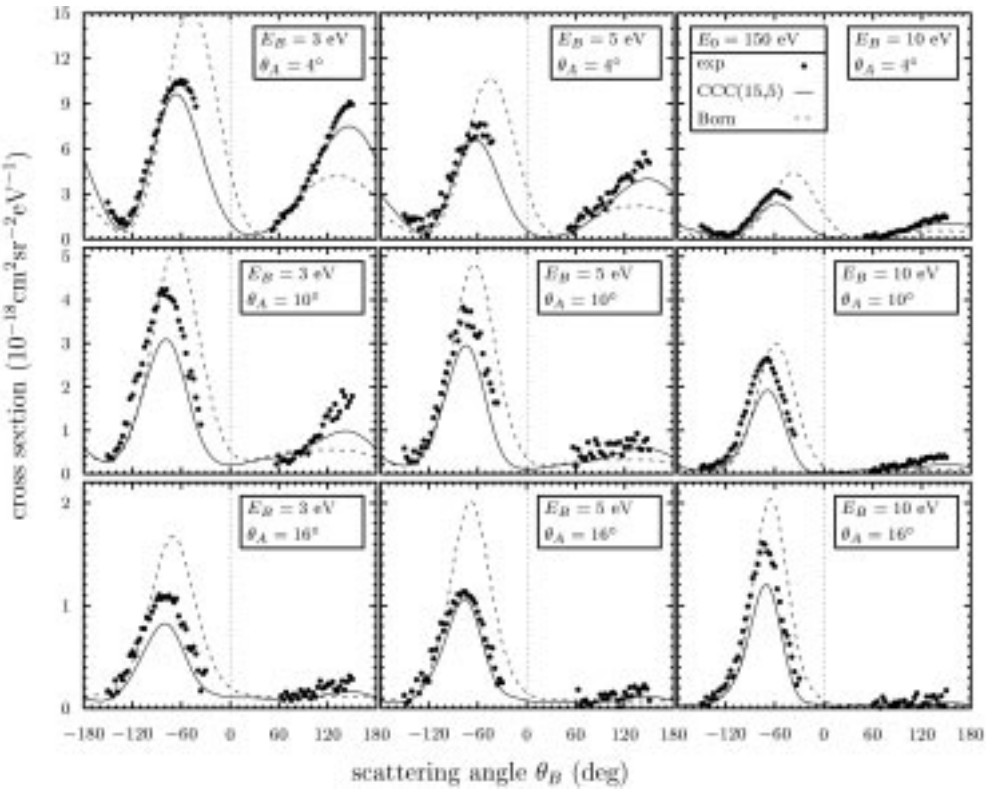

Fig. 9. Coplanar triply differential cross sections of the indicated electron of energy E_B with the E_A electron being detected at specified θ_A scattering angle for 150 eV electron-impact ionisation of the ground state of atomic hydrogen. The absolute measurements are due to Ehrhardt *et al.* (1986).

angles. The fact that these data lead to only a 30% lower TICS than the Shah *et al.* 1987 data is due to the $\sin\theta$ term in the integration of the DDCS to obtain the SDCS.

The TDCS are presented in Fig. 9. The difference between the Born and the CCC calculation is quite substantial. Comparison with the CCC(15,5) no exchange calculation indicates that the difference with the Born approximation is primarily due to coupling. The agreement with experiment is somewhat mixed. The fact that the Born approximation is too high and sometimes the CCC result too low indicates that a calculation which combines the two ideas, like a distorted-wave Born approximation (DWBA), may occasionally yield a better agreement with experiment than the CCC calculations presented; see Bray *et al.* (1994) for a comparison with other theory. However, we suppose that the present calculations should be the most accurate.

(3c) Incident Electron Energy 54·4 eV

This energy was also considered in the very first application of the CCC method to differential ionisation cross sections (Bray *et al.* 1994). However, as described in the previous subsection the formalism is now a little different, and also some new interesting issues have since emerged.

At 54·4 eV incident electron energy, absolute experimental TDCS for $E_B = 5$ eV exist for four angles of the fast electron (Röder *et al.* 1996*c*). We again apply a CCC(15,5) approximation at this energy. The energy levels of this calculation are given in Fig. 10. The energy distribution is much the same as at 250 and

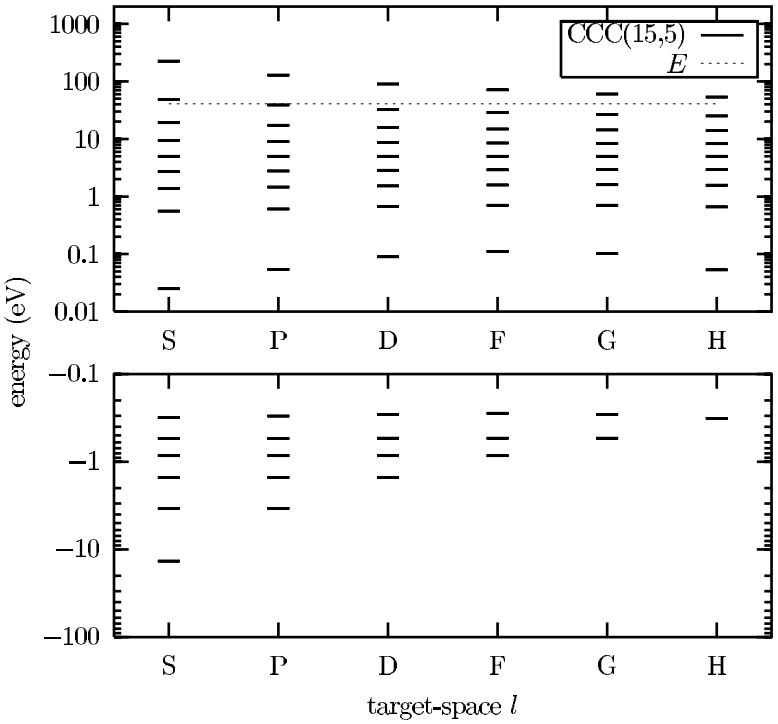

Fig. 10. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 54·4 eV e–H calculation using the CCC(15,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was 5 eV.

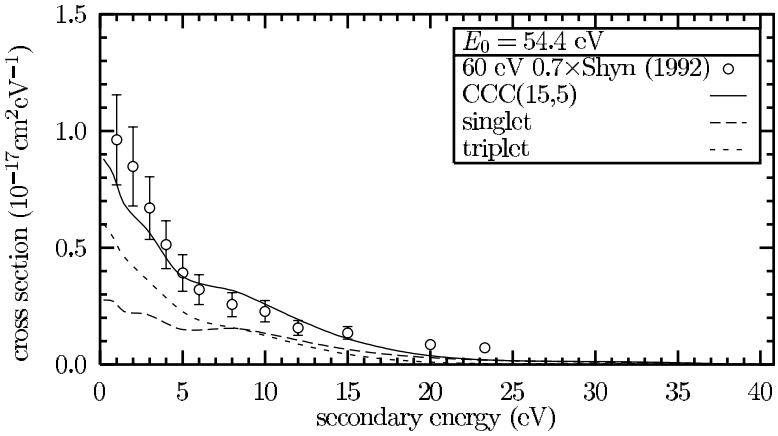

Fig. 11. Singly differential cross section for 54·4 eV electron-impact ionisation of the ground state of atomic hydrogen. The data of Shyn (1992) have been scaled for consistency with the data of Shah *et al.* (1987), see Fig. 1. The singlet and triplet contributions include the spin weights.

150 eV. The total energy $E = 54{\cdot}4$–$13{\cdot}6$ eV is such that there is a 'closed' state for each l (two for S-states). Bray and Clare (1997) discussed, by reference to the equivalent quadrature idea, the importance of having the total energy bisect two of the pseudothresholds. This is particularly important for small N_0 and E. Unfortunately, we are unable to have both an energy level at 5 eV and ensure that E is in between two other energy levels. In the present case this is not a major issue as we shall see that the SDCS is very small at the larger secondary energies.

In Fig. 11 the SDCS arising from the calculation is considered with comparison of the available rescaled 60 eV data of Shyn (1992). At this energy the Born approximation is much too high and we shall not consider it again. Instead, we shall concentrate on the importance of the two spin ($S = 0, 1$) channels. These are presented with the spin weights included so the spin-averaged sum is simply the sum of the singlet and triplet components.

Comparison with experiment is generally good, but looking at the individual spin components suggests the existence of a numerical problem. Whereas the triplet component is very smooth, the singlet one shows minor unphysical oscillation. It is our opinion that this is due to the fact the singlet SDCS at $E/2 = 20{\cdot}4$ eV is substantially bigger than the triplet one, which is near zero. If, as we suppose, the step-function hypothesis (Bray 1997) is true, then the size of the step should be relatively bigger for the singlet case. A finite discretisation of such a step function may be the cause of the oscillation. As a consequence, there is some uncertainty in the magnitudes of the singlet contribution at 5 eV. We could attempt to rescale the SDCS. However, at this energy we did not ensure an energy point at $E/2$ for each l, see Fig. 10. Hence the magnitude of the SDCS($E/2$) may significantly depend on the choice of interpolation.

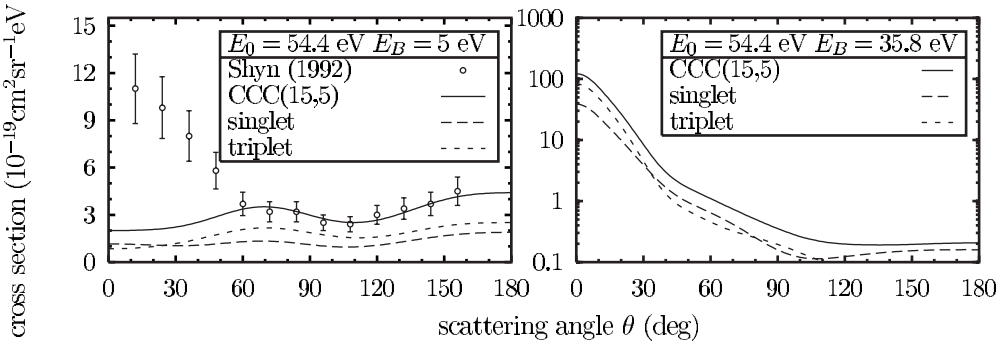

Fig. 12. Doubly differential cross section of the indicated outgoing electrons for $54{\cdot}4$ eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet contributions include the spin weights.

The DDCS are given in Fig. 12. Unscaled data of Shyn (1992) are compared with the CCC calculations. Also given are the singlet and triplet components. The agreement with experiment is good at intermediate and backward angles, but the systematic problem at forward angles continues.

The TDCS are presented in Fig. 13. For clarity of presentation we do not compare with the multitude of other available theories here. Considerable

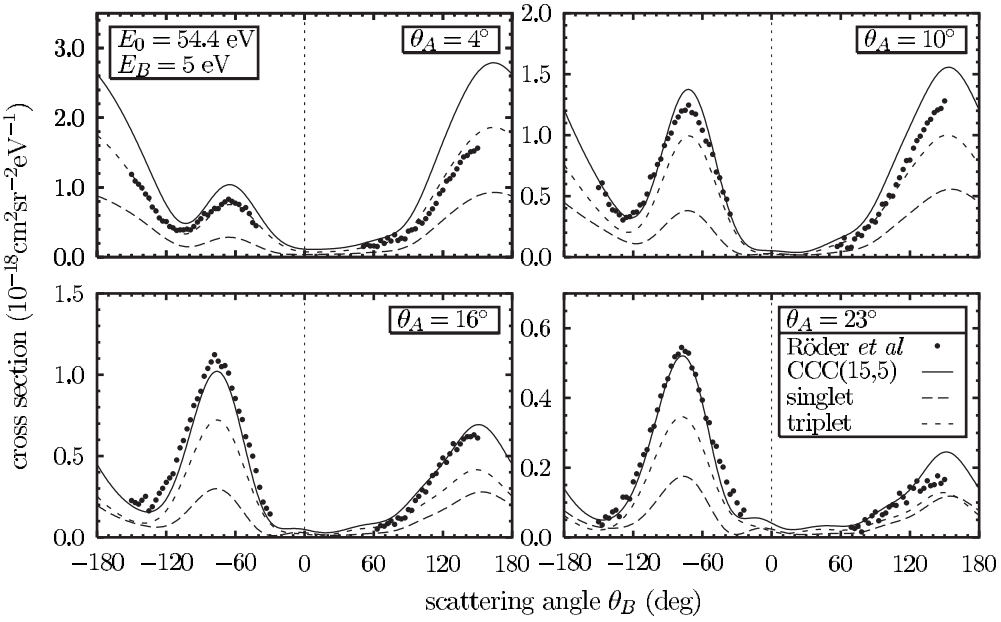

Fig. 13. Coplanar triply differential cross sections of $E_B = 5$ eV electrons for 54·4 eV electron-impact ionisation of the ground state of atomic hydrogen. The absolute measurements are due to Röder *et al.* (1996*c*).

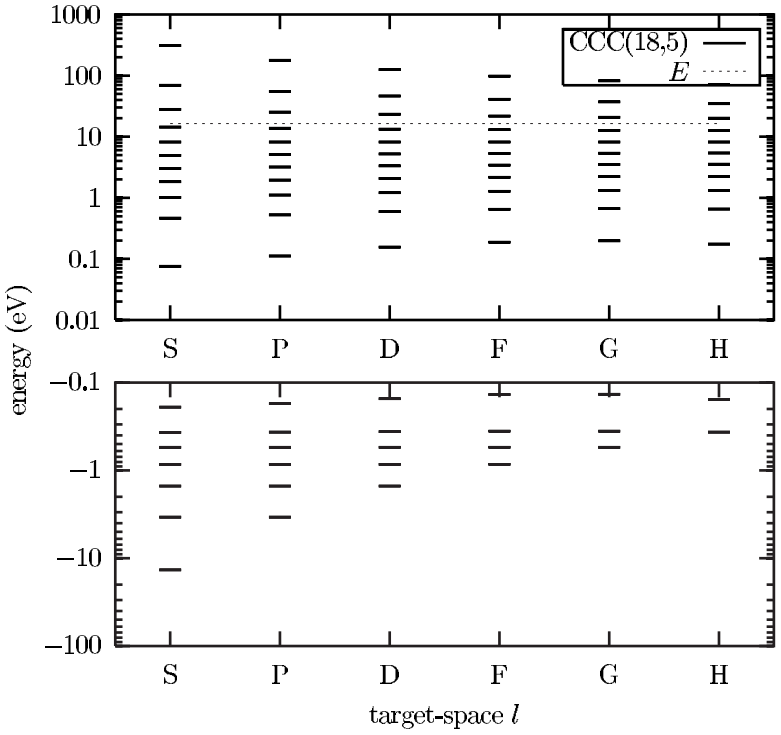

Fig. 14. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 30 eV e–H calculation using the CCC(18,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was 8·2 eV.

comparison of other theories with experiment may be found in Bray *et al.* (1994), Röder *et al.* (1996*c*) and Jones *et al.* (1997). The agreement with experiment is a little disturbing for small θ_A, but improves rapidly with increasing θ_A. Perhaps a more accurate theoretical estimate may be obtained by marginally increasing the singlet component (systematically for all θ_A), according to the discussion relating to the SDCS. Looking at the data it is difficult to argue for or against this case. What is clear is that due to the inherent difficulties of the CCC formalism e–H ionisation and e–He ionisation have different problems in terms of comparison with experiment. In the e–He case there is only one value of spin, here we have two, but experiment only measures their spin-averaged sum. These issues become more transparent at lower energies with equal energy-sharing kinematics.

(3d) Incident Electron Energy 30 eV

At 30 eV incident energy, relative equal energy-sharing ($E_B = E_A = 8{\cdot}2$ eV) data exist for the coplanar fixed θ_{AB} geometries (Röder *et al.* 1996*c*) and the coplanar symmetric geometry (Whelan *et al.* 1994). As the incident energy and hence E is reduced we need to take more care that E is nearly in between two of the pseudothresholds so that the integration rule associated with the open pseudostates ended near E. This issue is alleviated by having a larger N_0 as then the size of the SDCS at larger secondary energies is further reduced. For these reasons here we present the results of a CCC(18,5) calculation. The energy levels of this calculation are given in Fig. 14. The total energy $E = 16{\cdot}4$ eV is such that there are three 'closed' states for each l. Of the extra [over CCC(15,5)] three states for each l one has gone into the discrete spectrum and two into the continuum.

In Fig. 15 the SDCS arising from the CCC(18,5) calculation is considered. No experimental SDCS are available at this energy. At this energy the SDCS at $E/2$ is quite substantial, and thus we see unphysical oscillations in both the singlet and triplet components, though integrals of both yield excellent

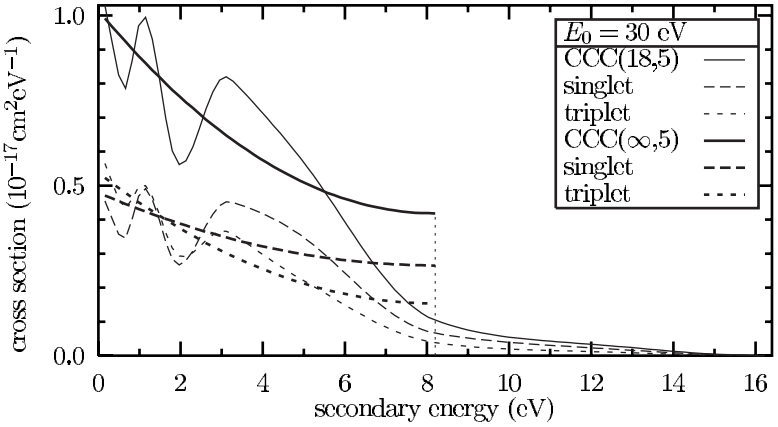

Fig. 15. Singly differential cross section for 30 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet results are obtained directly from the CCC(18,5) calculation (cf. equation 9). The CCC$(\infty, 5)$, singlet and triplet, curves are integral preserving estimates with CCC$(\infty, 5) = 4\times$CCC(18,5) at $E/2$, see text. The singlet and triplet contributions include the spin weights.

agreement with experiment, see Fig. 1. The unphysical oscillations indicate that the angular distributions will have incorrect magnitudes. We suppose that the integral preserving quadratic estimate labelled by CCC$(\infty, 5)$ is the step-function that the close-coupling formalism would converge to for infinite N_0. Convergence at exactly $E/2$ is to a quarter the height of the step, and is readily obtained in finite calculations, as we shall see at the next energy considered. Incidentally, the convergence in the SDCS with increasing $l_{\max}$ is particularly fast, and a CCC(18,3) calculation gives an almost indistinguishable SDCS result.

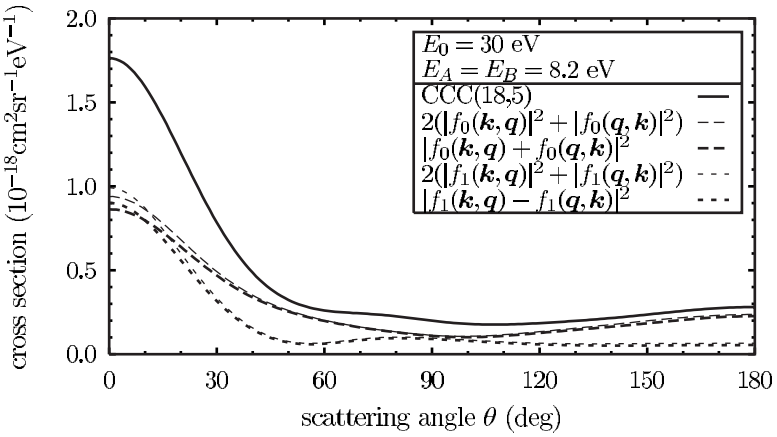

Fig. 16. Doubly differential cross section of the $8{\cdot}2$ eV outgoing electrons for 30 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet contributions include the spin weights, and have been evaluated using both sides of (27) prior to integration over one of the $d\Omega$.

The 30 eV DDCS, spin-weighted and the individual singlet and triplet components, are given in Fig. 16. These are given only for completeness as no experiment is yet available for this case. The singlet and triplet components evaluated using both sides of (27) are given to show the minimal difference between the two prescriptions.

The corresponding TDCS are presented in Fig. 17. The coplanar relative θ_{AB} measurements of Röder *et al.* (1996*c*) have been scaled by a single factor for best overall visual fit. The DWBA with polarisation and PCI effects calculation, presented in arbitrary units by Röder *et al.* (1996*c*), has been scaled to fit experiment as done by Röder *et al.* (1996*c*). In order to internormalise the coplanar symmetric data presented by Whelan *et al.* (1994) we have extracted the symmetric geometry points from the θ_{AB} measurements. The symmetric geometry calculation of Whelan *et al.* (1994) is internormalised to the θ_{AB} calculations, and is the reason why it is substantially higher than experiment compared to the initial presentation (Whelan *et al.* 1994).

The first thing to note is the excellent agreement between the coherent and incoherent combinations of amplitudes for both spins. The corresponding thick and thin curves are almost indistinguishable. There are some examples where the difference is quite visible. For the $\theta_{AB} = 150^\circ$ case around 0° and 160° there is approximately a 15% difference. However, the difference between the $|f_S(\boldsymbol{k},\boldsymbol{q})|^2$

and $|f_S(\boldsymbol{q},\boldsymbol{k})|^2$ components (not plotted) is around 50%. It is due to (26) applied to (27) that allows for such good agreement between the coherent and incoherent prescriptions.

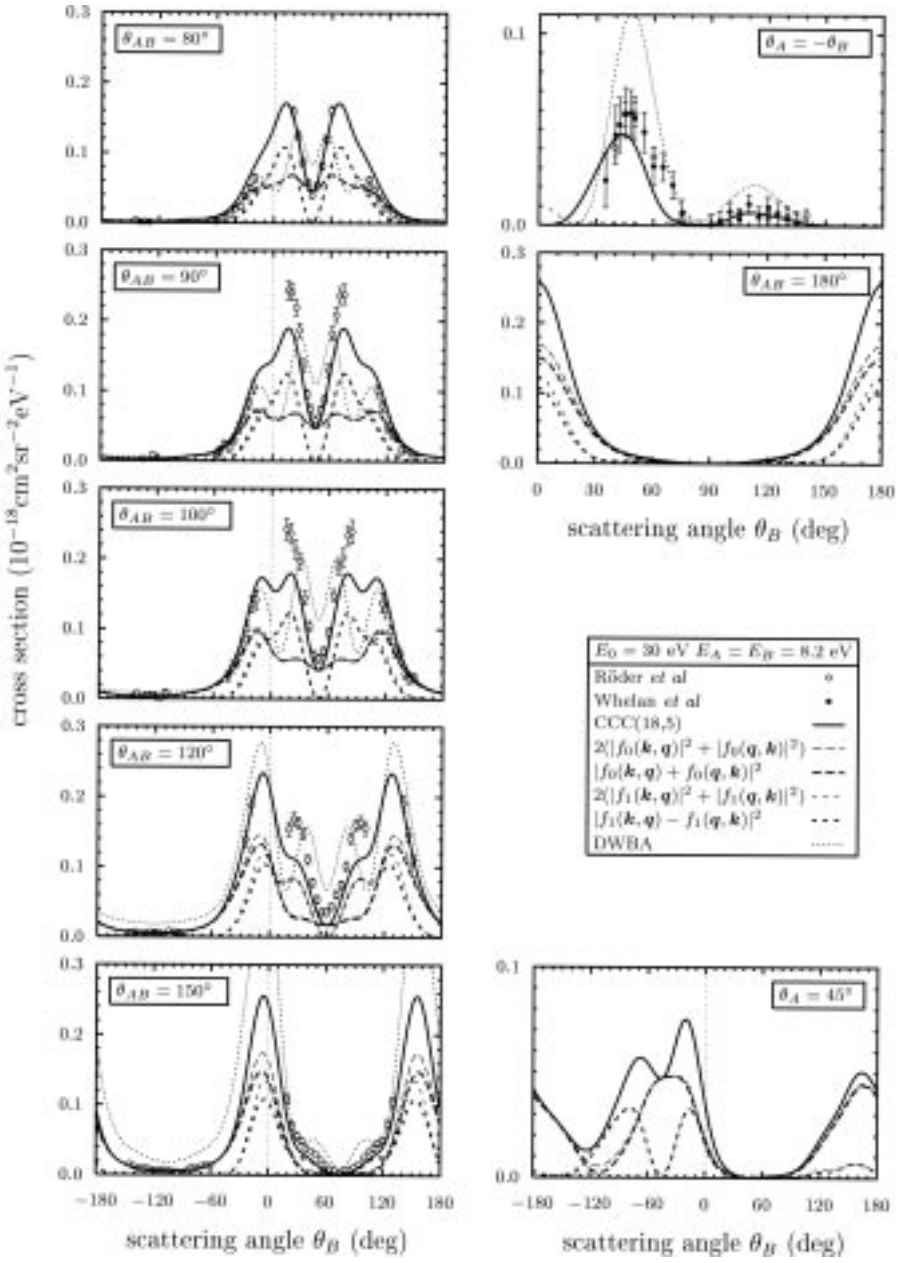

Fig. 17. Coplanar equal energy-sharing triply differential cross sections for 30 eV electron-impact ionisation of the ground state of atomic hydrogen. The internormalised relative θ_{AB} measurements, due to Röder *et al.* (1996*c*), have been normalised by a single factor to the CCC(18,5) calculation, whose singlet and triplet components are given according to (27). The measurements and calculations of Whelan *et al.* (1994) are internormalised with those of Röder *et al.* (1996*c*).

Looking at the case $\theta_{AB} = 80°$ the agreement between the CCC theory and experiment appears satisfactory. However, increasing the difference between the two detectors by just 10° results in a large rise in the experimental TDCS in the region of 20° and 60°. This is not reproduced by either theory, both of which predict only a marginal increase in the TDCS. In going from $\theta_{AB} = 90°$ to $\theta_{AB} = 100°$ both theories and experiment predict a small increase in the TDCS, with the discrepancy in the 20° to 80° angular range remaining. Increasing θ_{AB} by 20° more results in the experimental TDCS at 20° and 70° to drop substantially in magnitude, similar to the CCC theory. Curiously, if all of the $\theta_{AB} = 90°, 100°, 120°, 150°$ measurements in the region of 20° to 120° degrees were reduced by a factor of $0{\cdot}7$ or so, very good agreement with the CCC theory would be obtained.

For variety we have also given results for the $\theta_A = 45°$ geometry. It is interesting since in the region of $\theta_B = -45°$ the singlet component goes through a maximum while the triplet goes to zero due to antisymmetry, resulting in a triply peaked spin-averaged TDCS.

The so-called doubly symmetric ($E_A = E_B$, $\theta_A = -\theta_B$) geometry provides a good overall test of how well the CCC formalism is working. The two terms in (20) are identical (TDCS has a $\cos\theta$ dependence and hence independent of $\pm\theta$). The triplet amplitude should be identically zero at all angles due to the Pauli principle, while the singlet amplitude should be zero at forward and backward angles due to the electron–electron repulsion. Looking at this case we see that the triplet thin curve is near zero at most scattering angles, but rises at the forward angles. The coherent combination, on the other hand, yields identically zero for the triplet cross section as desired. To trace the source of the problem is quite simple. By generating the TDCS after each partial wave J of total orbital angular momentum we find that the forward triplet TDCS grows for $J > 5$. This is because exchange may only be treated properly between electron functions of same angular momentum. Given that we have $l_{\max} = 5$, for higher L of the projectile exchange cannot be fully implemented. Though presently not practical, for computational reasons, larger $l_{\max}$ would be necessary to obtain even smaller triplet TDCS.

Overall, we find the agreement with experiment in this case somewhat disturbing. Here the excess energy is $16{\cdot}4$ eV. It is interesting to compare with the $44{\cdot}6$ eV e–He ionisation case, where the excess energy is 20 eV (Rioual *et al.* 1998). Generally much better agreement with experiment is found in this case, particularly at $\theta_{AB} = 90°$. Incidentally, the rescaling of the CCC theory in the latter case was independently found to be a factor of 2.

(3e) Incident Electron Energy 27·2 eV

This energy is particularly interesting due to experimental data being available at $E_B = 2$ eV (Berakdar *et al.* 1996), $E_B = 4$ eV (Ehrhardt and Röder 1997) and $E_B = E_A = 6{\cdot}8$ eV (Brauner *et al.* 1991*b*) secondary energies. Unfortunately, the data are relative and may not be related across the energy-sharing. This case has been recently studied by Jones and Madison (1998) and Berakdar *et al.* (1999). The latter presented the 3C, DS3C and a CCC(15,5) calculation, and suggested that the calculations of Jones and Madison (1998) may be much too low. Here we present the results of a CCC(18,5) calculation. Its results are

compared to those of the CCC(15,5) calculation to test both the convergence and the rescaling prescription.

The energy levels of this calculation are given in Fig. 18. They differ substantially from those used in the CCC(15,5) calculation (Berakdar *et al.* 1999),

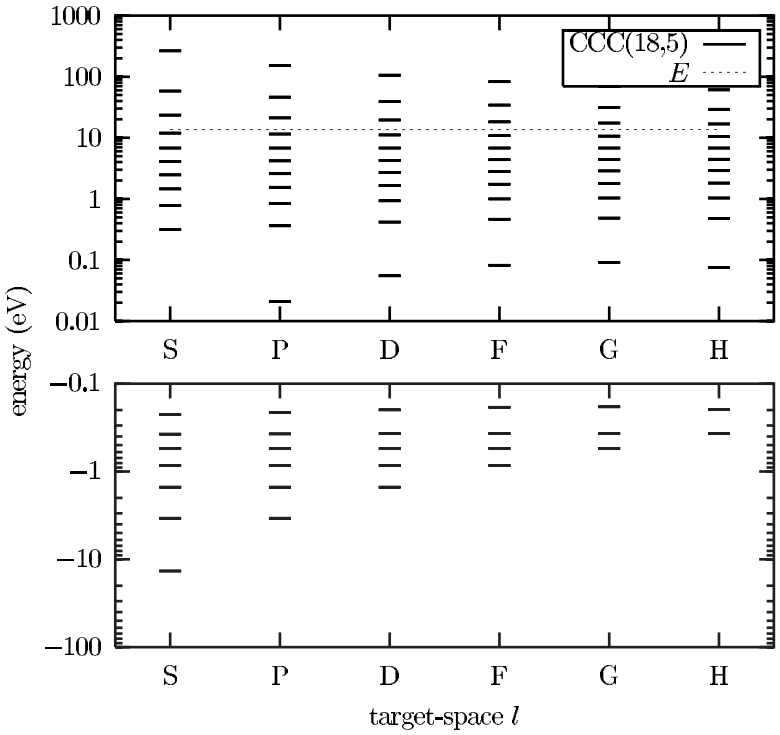

Fig. 18. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 27·2 eV e–H calculation using the CCC(18,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was 6·8 eV.

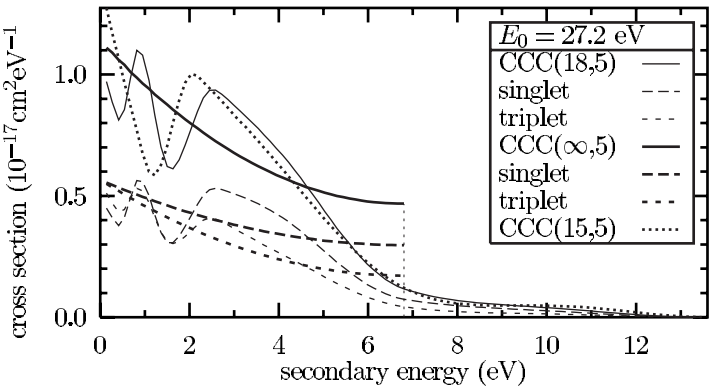

Fig. 19. Singly differential cross section for 27·2 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet (spin weights included) results are obtained directly from the CCC(18,5) calculation (cf. equation 9). The CCC(∞, 5) curve is an integral preserving estimate, see text. The CCC(15,5) curve is from Berakdar *et al.* (1999). The ratios of CCC(∞, 5) to CCC(18,5) at 2, 4 and 6·8 eV are 1·0, 0·8 and 4.

and thus provide for a particularly good test of the CCC formalism for increasing N_0. The λ_l were chosen so that one of the energies was equal to $6{\cdot}8$ eV for each l.

In Fig. 19 the SDCS arising from the CCC(18,5) calculation are considered. No experimental SDCS are available at this energy, but we compare with the SDCS arising from the CCC(15,5) calculation (Berakdar *et al.* 1999). The discussion of the 30 eV SDCS is equally applicable here, including the estimation of CCC$(\infty, 5)$. Some difference can be seen between the CCC(18,5) and CCC(15,5) SDCS, with the former showing more oscillation than the latter. Yet the two SDCS are nearly identical at $E/2$.

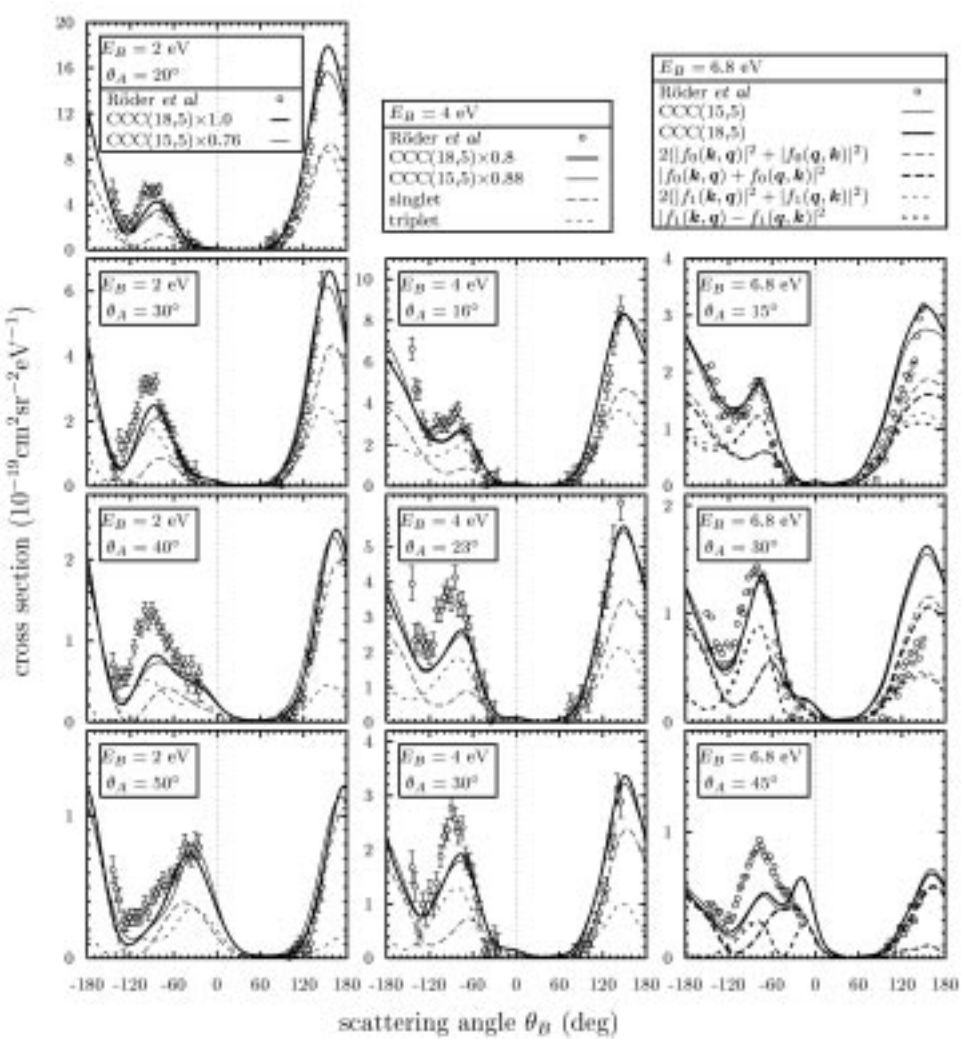

Fig. 20. Coplanar triply differential cross sections for $27{\cdot}2$ eV electron-impact ionisation of the ground state of atomic hydrogen. The internormalised relative E_B =2, 4 and $6{\cdot}8$ eV measurements are from Berakdar *et al.* (1996), Ehrhardt and Röder (1997) and Brauner *et al.* (1991*b*) respectively. The measurements have been normalised using a single E_B-dependent factor, to the CCC(18,5) calculation. The CCC(15,5) TDCS is from Berakdar *et al.* (1999), however at $6{\cdot}8$ eV, like the CCC(18,5) TDCS, has been obtained using the right side of (27).

The corresponding TDCS are presented in Fig. 20. We see that in all cases the agreement between the two CCC calculations is very good, confirming the claim of relatively fast convergence in the angular distributions generally, and absolute values, so long as account is taken that convergence of the raw CCC results at $E/2$ is to half the true magnitude, with subsequent rescaling. The calculations presented are also a good check of the internal interpolation (Bray and Fursa 1996*a*) which is necessary in both calculations for $E_B = 2$ and 4 eV.

Though the CCC-calculated TDCS have converged (again $l_{\max} = 5$ is sufficient) in both shape and magnitude (after rescaling), the occasional substantial discrepancy with experiment is disturbing. A case we would like to single out is for $E_B = E_A, \theta_A = 45°$. Here, as at 30 eV, around $\theta_B = -45°$ the singlet TDCS goes through a maximum while the triplet TDCS goes through zero. This leads to a triply peaked CCC-calculated TDCS, contrary to the experimental finding. Furthermore, the DS3C calculation (see Berakdar *et al.* 1999) is in much better agreement with experiment than the CCC calculations. We have no explanation for this. Since (27) is well-satisfied the problem is not due to symmetry problems in the amplitudes. Whereas agreement with experiment is satisfactory at $\theta_A = 15°$ and $\theta_A = 30°$, such a discrepancy for $\theta_A = 45°$ is surprising. For other cases the agreement with experiment is generally satisfactory.

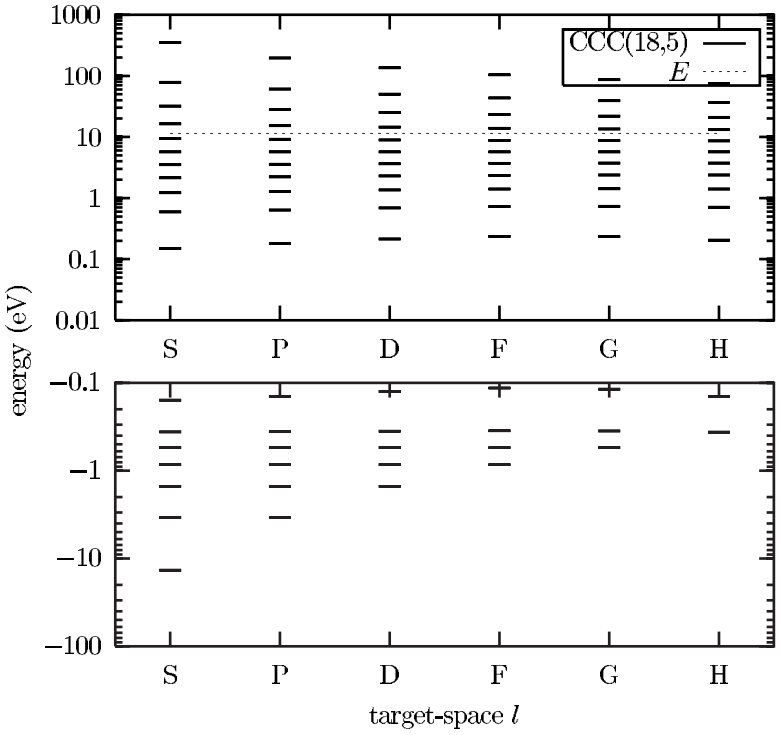

Fig. 21. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 25 eV e–H calculation using the CCC(18,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was $5{\cdot}7$ eV.

(3f) Incident Electron Energy 25 eV

At 25 eV coplanar equal energy-sharing relative fixed θ_{AB} data are available (Röder *et al.* 1996*c*), as well as for the symmetric geometry (Whelan *et al.* 1994). In Fig. 21 the energy levels of the CCC(18,5) calculation are presented. For each l there is a state with energy $E/2 = 5 \cdot 7$ eV.

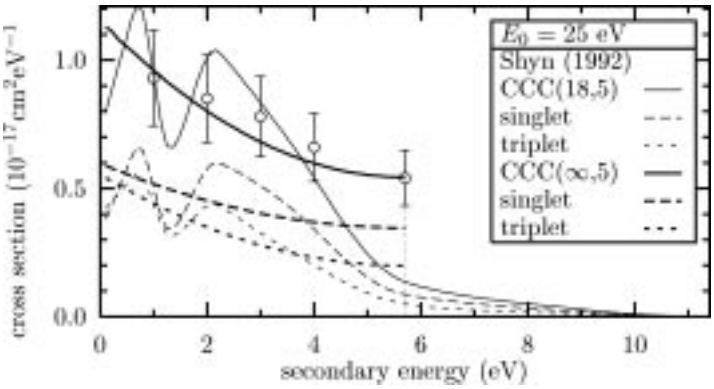

Fig. 22. Singly differential cross section for 25 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet results are obtained directly from the CCC(18,5) calculation (cf. equation 9). The CCC$(\infty, 5)$ curve is an integral preserving estimate, see text. The singlet and triplet contributions include the spin weights.

In Fig. 22 the SDCS arising from the CCC(18,5) calculation are considered and compared with the data of Shyn (1992). Once again the discussion of the 30 eV SDCS is equally applicable here. We see good agreement of the CCC$(\infty, 5)$ estimate (see above) with the experimental data, which at this energy has not been rescaled as it is already in agreement with the data of Shah *et al.* (1987), see Fig. 1.

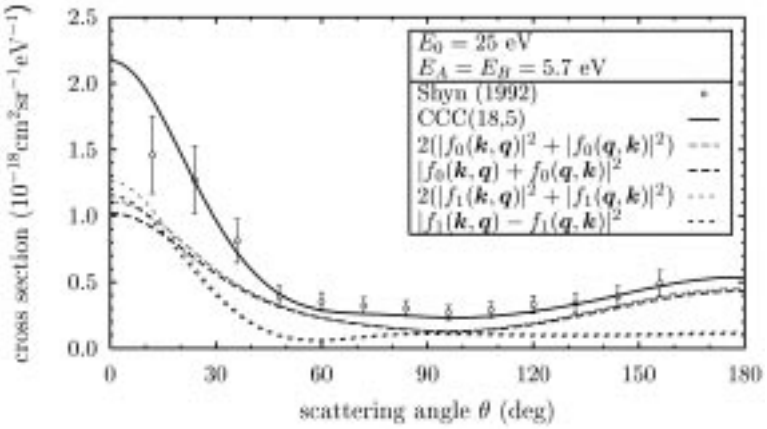

Fig. 23. Doubly differential cross section of the $5 \cdot 7$ eV outgoing electrons for 25 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet contributions include the spin weights, and have been evaluated using both sides of (27) prior to integration over one of the $d\Omega$.

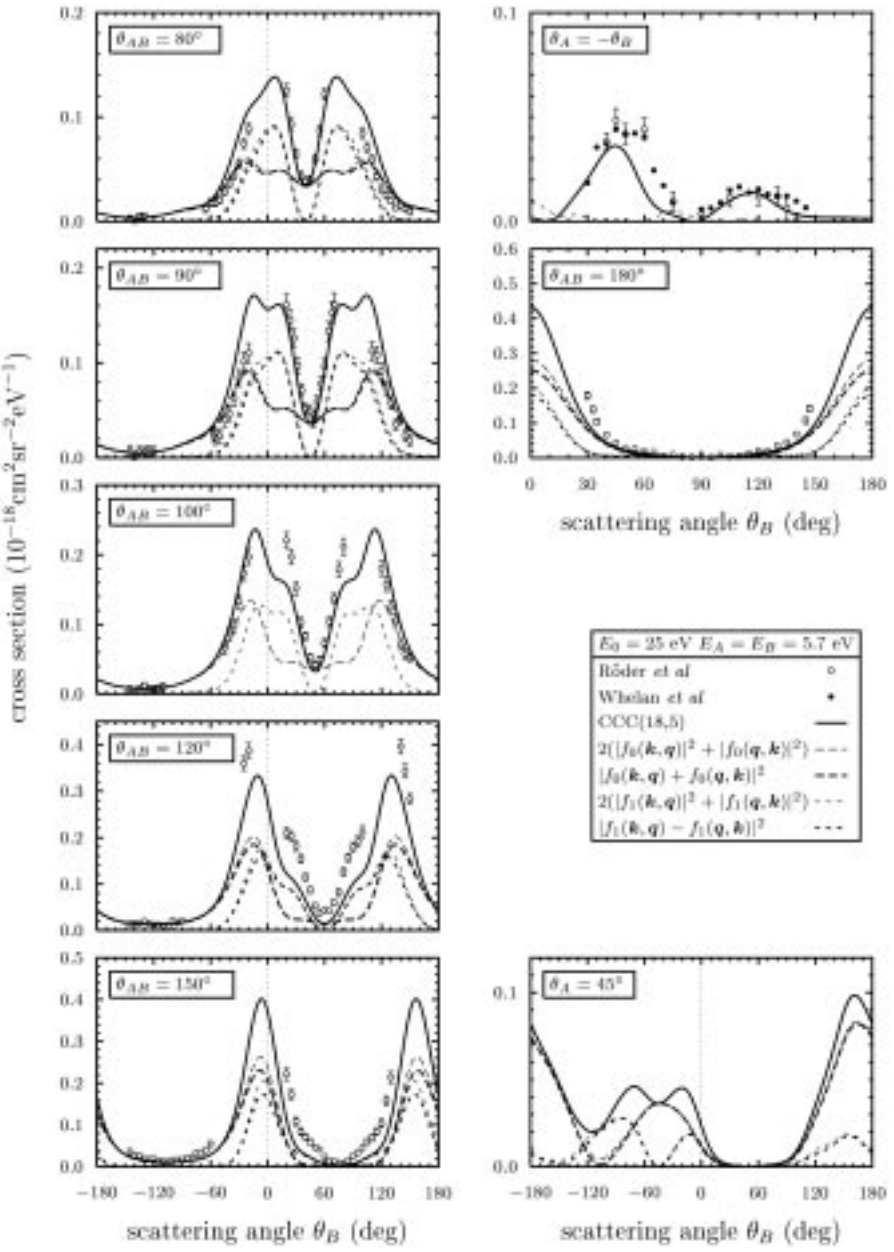

Fig. 24. Coplanar equal energy-sharing triply differential cross sections for 25 eV electron-impact ionisation of the ground state of atomic hydrogen. The internormalised relative θ_{AB} measurements, due to Röder *et al.* (1996*c*), have been normalised by a single factor to the CCC(18,5) calculation, whose singlet and triplet (with weights) components are evaluated using (27). The measurements presented by Whelan *et al.* (1994) are internormalised with those of Röder *et al.* (1996*c*).

The 25 eV DDCS are given in Fig. 23 and are compared with experiment. This time we find complete agreement with experiment. Why this should be so at this, relatively low, energy and not at higher ones is a somewhat surprising, and may be coincidental. Once again very good agreement between the two sides of (27) is found for both the singlet and triplet components.

The TDCS are presented in Fig. 24. The coplanar relative θ_{AB} measurements of Röder *et al.* (1996*c*) have been scaled by a single factor for best overall visual fit to the theory. In order to internormalise the coplanar symmetric data presented by Whelan *et al.* (1994) we have extracted the symmetric geometry points from the θ_{AB} measurements. The general agreement with experiment is not too bad. The transition from $\theta_{AB} = 80°$ to $\theta_{AB} = 90°$ is now more consistent than in the case of 30 eV incident energy. Interestingly, as at 30 eV, a systematic reduction of the measurements in the 20°–80° region relative to others would result in even better agreement with experiment. The decomposition of the CCC results into their singlet and triplet components is helpful to check the accuracy of the coherent versus incoherent combinations of the CCC amplitudes, see equation (27).

(3g) Incident Electron Energy 20 eV

The availability of the 20 eV incident energy measurements is much the same as for the 30 and 25 eV cases. Coplanar data are available for equal energy-sharing relative fixed θ_{AB} and symmetric geometries (Röder *et al.* 1996*c*; Whelan *et al.* 1994).

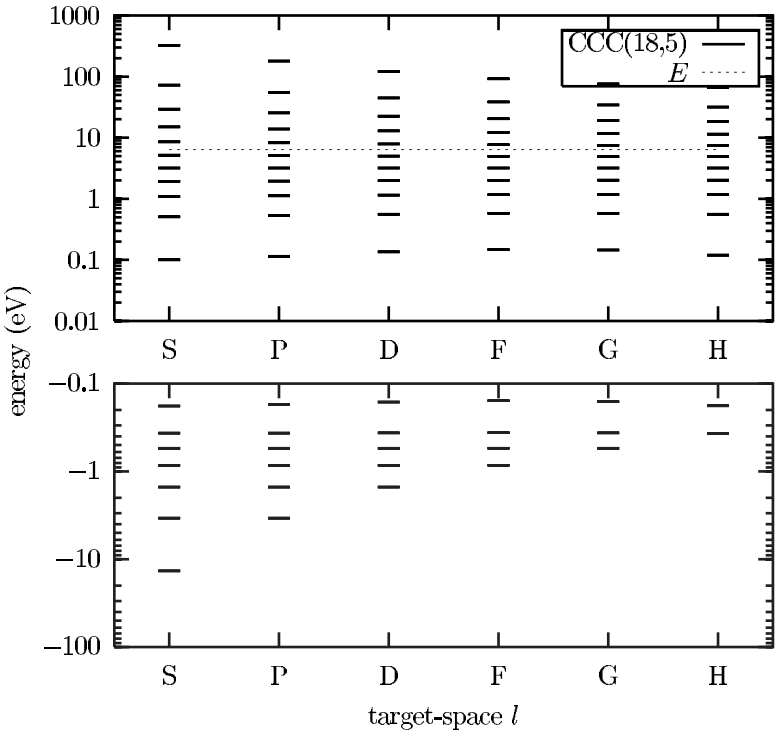

Fig. 25. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 20 eV e–H calculation using the CCC(18,5) model with $\lambda_l \approx 1{\cdot}0$. The λ_l were chosen so that for each l one energy was $3{\cdot}2$ eV.

In Fig. 25 the energy levels of the CCC(18,5) calculation are presented, where this time there is a state of energy $3 \cdot 2$ eV for each l. The SDCS arising from the CCC(18,5) calculation are presented in Fig. 26. We see that the triplet component is now systematically lower than the singlet, with both showing similar unphysical oscillations. The two given integral preserving quadratic estimates of the SDCS are not used in the present calculations since data are only available for the equal-energy-sharing kinematical region.

The 20 eV DDCS are given in Fig. 27. No experiment is yet available, and so we present it for completeness in the hope that this work will generate some interest in measuring these fundamental cross sections on a broad energy range.

The TDCS are presented in Fig. 28. As at 30 and 25 eV the relative constant θ_{AB} measurements of Röder *et al.* (1996*c*) have been scaled by a single factor

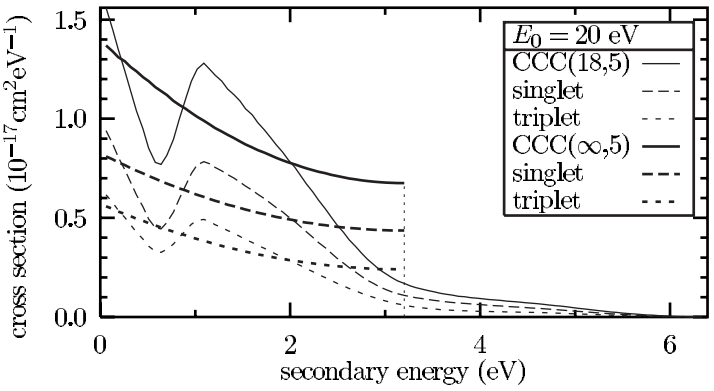

Fig. 26. Singly differential cross section for 20 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet results are obtained directly from the CCC(18,5) calculation (cf. equation 9). The CCC$(\infty, 5)$ curve is an integral preserving estimate, see text.

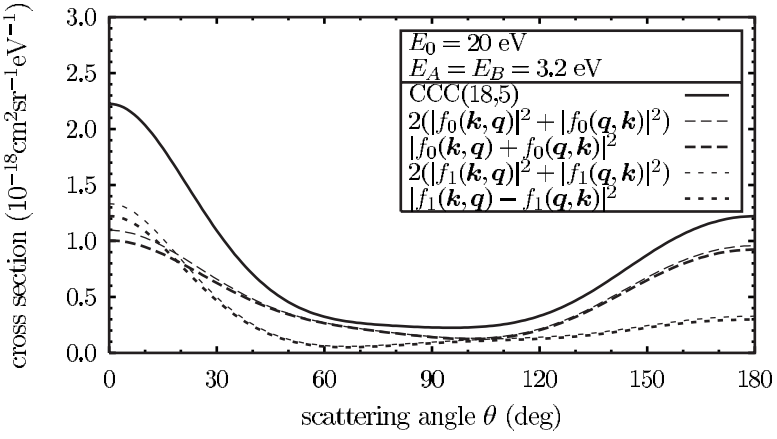

Fig. 27. Doubly differential cross section of the $3 \cdot 2$ eV outgoing electrons for 20 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet contributions include the spin weights, and have been evaluated using both sides of (27) prior to integration over one of the $d\Omega$.

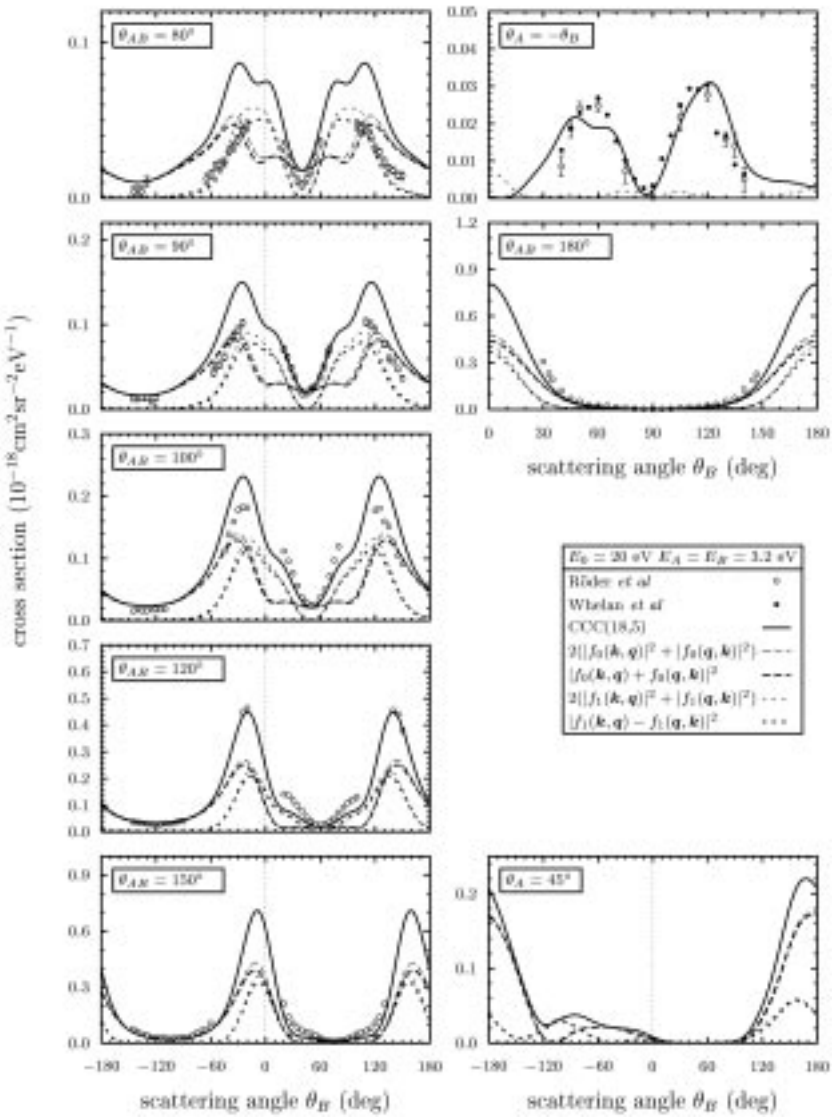

Fig. 28. Coplanar equal energy-sharing triply differential cross sections for 20 eV electron-impact ionisation of the ground state of atomic hydrogen. The internormalised relative θ_{AB} measurements, due to Röder *et al.* (1996*c*), have been normalised by a single factor to the CCC(18,5) calculation, whose singlet and triplet (with weights) components have been evaluated using (27). The measurements, presented by Whelan *et al.* (1994), have been internormalised with those of Röder *et al.* (1996*c*).

for best overall visual fit to the CCC(18,5) theory. In order to internormalise the symmetric data (Whelan *et al.* 1994) we have extracted the symmetric geometry points from the θ_{AB} measurements. We see that for the smaller θ_{AB} there is a major problem. Though the shape of theory and experiment is generally quite similar there is significant discrepancy in magnitude. We wonder if the experimental internormalisation is at least partially responsible for the discrepancy.

For small $E_A = E_B$ and small θ_{AB} the TDCS are particularly small, and it would be helpful to have a number of fixed θ_A geometries measured to check the consistency of the internormalisation. Because of the substantial discrepancies we performed many calculations which included CCC(18,4) and CCC(20,5) models. These yield barely different results, in shape and magnitude, to those presented. We acknowledge certain numerical difficulties with the presented calculations as can be observed from the non-zero triplet TDCS for the symmetric geometry calculated using the incoherent combination of amplitudes. However, we do not believe they are the cause of the substantial discrepancies observed here, since generally the agreement between the two sides of (27) is very good.

(3h) Incident Electron Energy 17·6 eV

We now approach the near threshold region of e–H ionisation. Here absolute TDCS are available (Röder *et al.* 1997*b*). Furthermore, the data are very detailed in that both fixed θ_A and θ_{AB}, as well as symmetric geometries have been measured. As before, all of the data are coplanar.

In Fig. 29 the energy levels of the CCC(20,5) calculation are presented. The value of N_0 has been increased and the λ_l decreased in order to get a more accurate description of the kinematic region below the $E = 4$ eV total energy. We also performed many smaller calculations which show marginal difference to the largest presented.

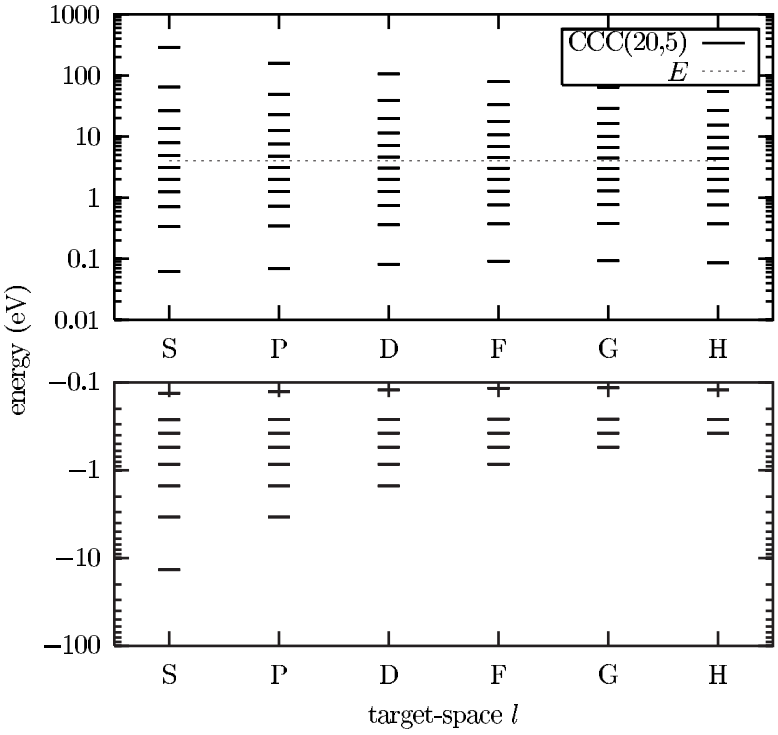

Fig. 29. Energy levels $\epsilon_{nl}^{(N)}$ arising in the 17·6 eV e–H calculation using the CCC(20,5) model with $\lambda_l \approx 0{\cdot}8$. The λ_l were chosen so that for each l one energy was 2 eV.

In Fig. 30 the SDCS arising from the CCC(20,5) calculation are considered. We see that the triplet component is now even lower than the singlet, showing similar but less pronounced unphysical oscillations.

For completeness the 17·6 eV DDCS are given in Fig. 31. It shows the unusual situation where forward and backward scattering are equally dominant.

The TDCS are presented in Fig. 32. In order to obtain best visual agreement of the rescaled CCC(20,5) calculations with experiment as a whole the measurements were scaled by a factor of 0·5. This is a little outside the ±40% experimental uncertainty (Röder *et al.* 1997*b*).

As at 20 eV there are substantial discrepancies for the fixed small θ_{AB} geometries. This time it is not just a problem of internormalisation. The discrepancy around 60° is substantially smaller than at say 120°. It is particularly helpful to have

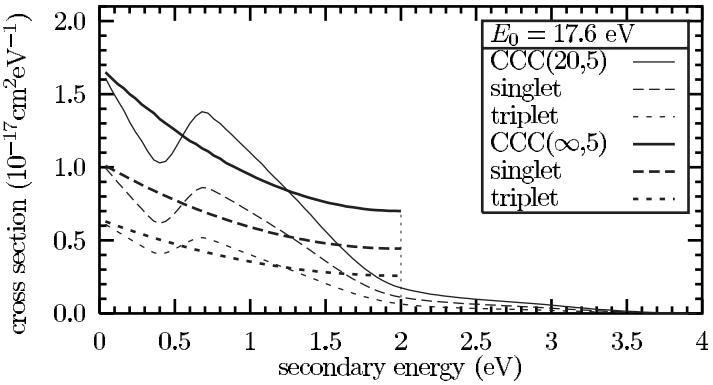

Fig. 30. Singly differential cross section for 17·6 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet results are obtained directly from the CCC(20,5) calculation (cf. equation 9). The CCC(∞, 5) curve is an integral preserving estimate, see text. The singlet and triplet contributions include the spin weights.

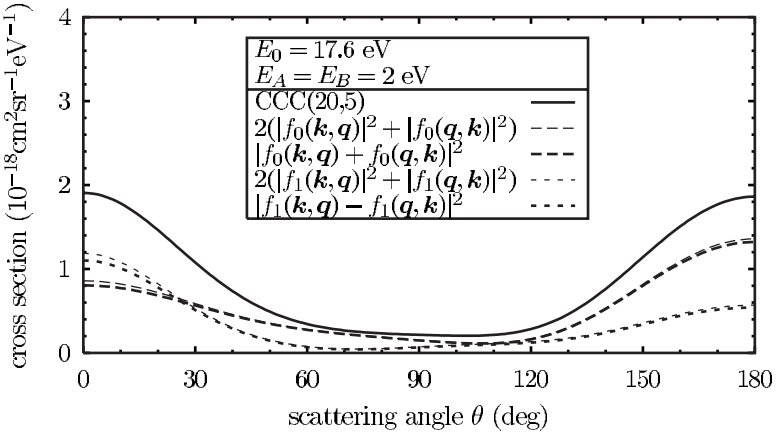

Fig. 31. Doubly differential cross section of the 2 eV outgoing electrons for 17·6 eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet contributions include the spin weights, and have been evaluated using both sides of (27) prior to integration over one of the $d\Omega$.

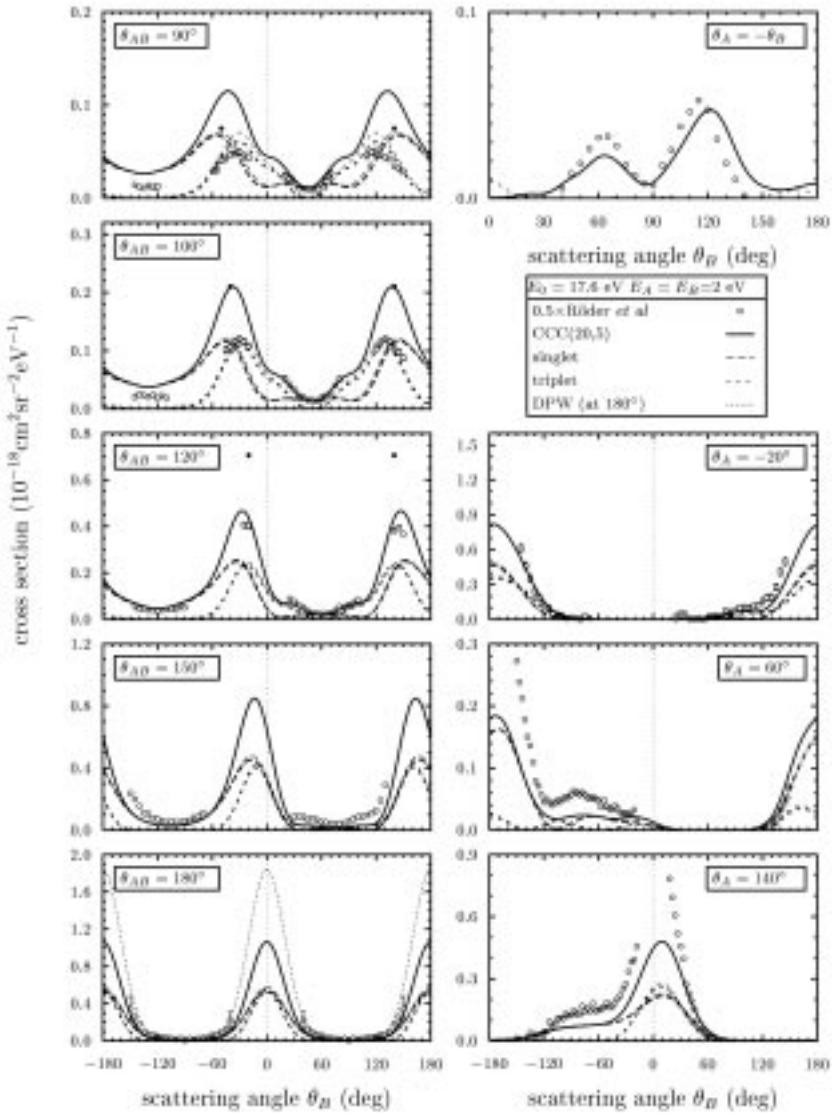

Fig. 32. Coplanar equal energy-sharing triply differential cross sections for 17·6 eV electron-impact ionisation of the ground state of atomic hydrogen. The open circles, denoting the absolute measurements of Röder *et al.* (1996*c*, 1997*b*), have been reduced by the 0·5 factor for best overall visual agreement to the CCC(20,5) calculation, whose singlet and triplet (with weights) components are given according to (27). The solid circles for the $\theta_{AB} = 90°, 100°, 120°$ are from the $\theta_A = 140°$ measurement for $\theta_B = 50°, 40°, 20°$, respectively. The distorted partial-wave (DPW) calculation is due to Pan and Starace (1992) and reported by Röder *et al.* (1997*b*).

so many different geometries measured. The symmetric geometry defines the relationship between the singlet theoretical component and the experiment. The discrepancy at backward $\theta_A = -\theta_B$ angles is responsible for the difference between experiment and theory in the region of $-120°$ for the $\theta_{AB} = 90°,\ 100°,\ 120°$

geometries. The singlet and triplet components evaluated according to (27) are in good agreement with each other generally. One exception is at forward angles of the symmetric geometry where the triplet TDCS evaluated using the left side of (27) is non-zero. The right side of (27) yields identically zero for the triplet cross section.

We are also able to check the internal consistency of the measurements by taking say the $\theta_A = 140^\circ$ measurements and plotting them at the appropriate points on the constant θ_{AB} plots. The solid circles are examples of this. We see substantial inconsistency of the measurements. The inconsistent improvement in the agreement between theory and experiment, by simply increasing a particular set of constant θ_{AB} measurements, implies that internormalisation is not the sole reason for the discrepancy between theory and experiment. We hope that the presented experimental inconsistency will lead to experimental reinvestigation of this incident energy.

Röder *et al.* (1997*b*) also presented the distorted partial-wave (DPW) calculation of Pan and Starace (1992), available only for $\theta_{AB} = 180^\circ$. Comparison of the CCC results with this calculation is also presented in Fig. 32. The CCC estimate is around $1{\cdot}5$ times lower than the DPW calculation.

(3i) Incident Electron Energy 15·6 eV

This energy was the subject of the preliminary investigation of this work (Bray 1999). We present these results here for completeness, to give more information

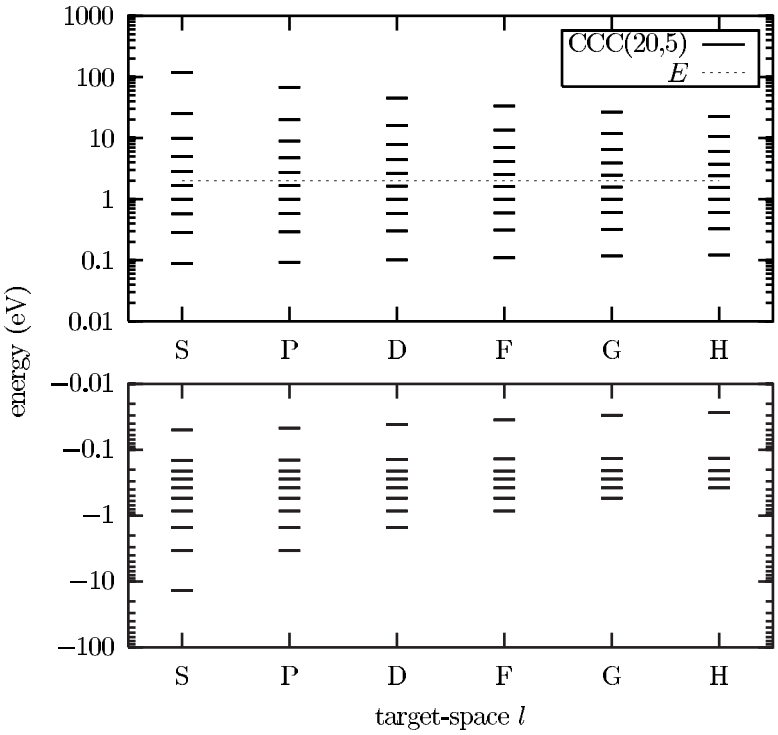

Fig. 33. Energy levels $\epsilon_{nl}^{(N)}$ arising in the $15{\cdot}6$ eV e–H calculation ($E = 2$ eV) using the CCC(20,5) model with $\lambda_l \approx 0{\cdot}6$. The λ_l were chosen so that for each l one energy was 1 eV.

and for ready contrast to other energies. Furthermore, the earlier results were rescaled up by a factor of $2 \cdot 7$ upon the assumption of a flat true SDCS. Here we obtain the magnitude ab initio, which indicates that the previous results should heve been scaled up by exactly a factor of 2. Hence, we believe that the e–H SDCS is still not flat at this energy.

The energies arising in the CCC(20,5) calculations are given in Fig. 33. The $\lambda_l \approx 0 \cdot 6$ have been reduced further in order to have more states of energy less than the 2 eV total energy. Though the ideal value of λ_0 for the 1S state is 2, with a basis size of 20 there is no difficulty in reproducing the 1S state even with $\lambda_0 \approx 0 \cdot 6$.

In Fig. 34 the SDCS arising from the CCC(20,5) calculation are considered. Also given is the spin-averaged SDCS of the CCC(13,4) calculation published

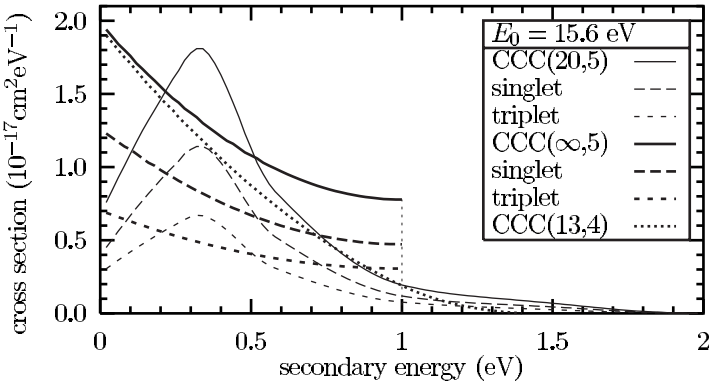

Fig. 34. Singly differential cross section for $15 \cdot 6$ eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet results are obtained directly from the CCC(20,5) calculation (cf. equation 9). The CCC$(\infty, 5)$ curve is an integral preserving estimate, see text. The singlet and triplet contributions include the spin weights. Both the CCC(20,5) and the CCC(13,4) are from Bray (1999).

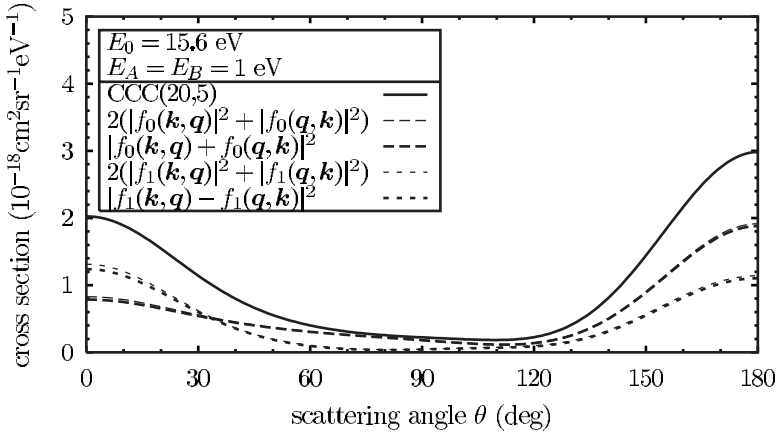

Fig. 35. Doubly differential cross section of the 1 eV outgoing electrons for $15 \cdot 6$ eV electron-impact ionisation of the ground state of atomic hydrogen. The singlet and triplet contributions include the spin weights, and have been evaluated using both sides of (27) prior to integration over one of the $d\Omega$.

earlier (Bray 1999). The two agree very well at the $E/2$ point, and yield a quarter of the true SDCS. Whereas previously we thought that this was an indication of extremely slow convergence, now we realise that convergence has been achieved in the CCC-calculated amplitudes, but to half the true magnitude. The shape of the CCC-calculated SDCS has changed substantially from the flat SDCS we supposed earlier (Bray 1999). Perhaps the work of Baertschy *et al.*

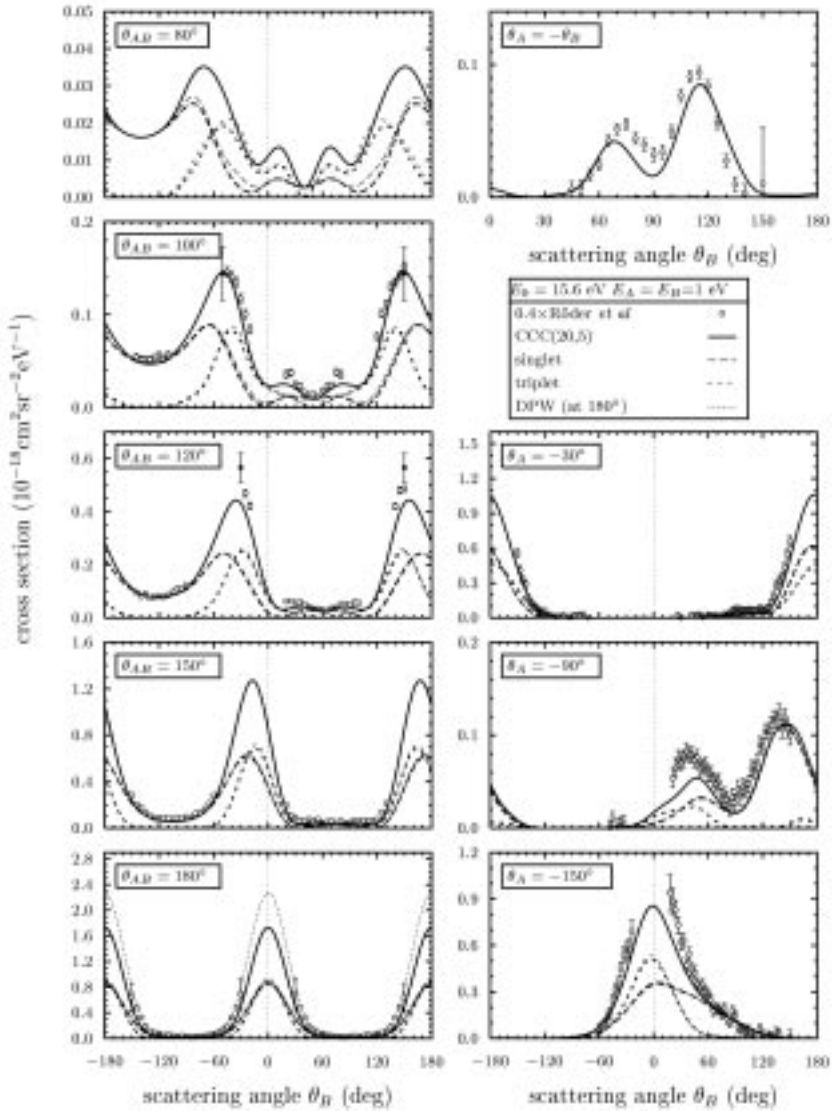

Fig. 36. Coplanar equal energy-sharing triply differential cross sections for $15{\cdot}6$ eV electron-impact ionisation of the ground state of atomic hydrogen. The absolute measurements are due to Röder *et al.* (1996*c*, 1997*b*). The solid circles for $\theta_{AB} = 100^\circ, 120^\circ$ geometries are from the $\theta_A = -150^\circ$ geometry with $\theta_B = -50^\circ, -30^\circ$ respectively. The internormalisation of the $\theta_{AB} = 100^\circ$ case has been changed from the original measurements to the $(\theta_A, \theta_B) = (-150^\circ, -50^\circ)$ (solid circle) point, see text. The CCC(20,5) calculation has been presented earlier (Bray 1999), but here is evaluated according to (27).

(1999) applied to the full e–H problem will give definitive SDCS that may be compared with the estimates given.

The 15·6 eV DDCS are given in Fig. 35. Remarkably we find that backward scattering is the most dominant.

The TDCS are presented in Fig. 36. In contrast to the slightly higher incident energies we find excellent agreement between theory and experiment, after the latter has been reduced by 0·4. We do note, however, that the original internormalisation of the $\theta_{AB} = 100^\circ$ measurements was not consistent with the $\theta_B = -50^\circ$ (solid) point of the $\theta_A = -150^\circ$ geometry. Accordingly, we imposed this internormalisation by scaling the $\theta_{AB} = 100^\circ$ measurements by a factor of 1·5 before plotting. The $\theta_{AB} = 120^\circ$ measurements are reasonably consistent with the $\theta_B = -30^\circ$ point of the $\theta_A = -150^\circ$ geometry.

The uniform reduction of the experiment by the factor of 0·4 is outside the stated ±35% uncertainty of the absolute value determination (Röder *et al.* 1997*b*). The true SDCS would have to be highly convex in order for the experimental absolute values to be correct. Recall that the CCC-calculated and estimated SDCS correctly yield the spin-dependent total ionisation cross sections at this energy (see Fig. 1).

4. Conclusions

An extensive and systematic study of e–H ionisation has been performed from 250 eV to 15·6 eV incident energy. It was shown how the close-coupling approach to ionisation converges to the Born approximation at high energies. While we believe it is common knowledge that exchange effects disappear at high energies, Bencze and Chandler (1999) argue that the treatment of exchange in our formalism should lead to amplitudes that satisfy the symmetrisation postulate and hence yield a symmetric SDCS. Their argument is independent of energy, and it is our view that this claim is incorrect. Instead, we still suspect to be true the step function hypothesis (Bray 1997), which states that with increasing N the CCC-calculated amplitudes should converge to zero on the secondary energy range of $[E/2, E]$, for all total energies E. The presented results are consistent with this idea, and the unphysical oscillations in the SDCS for small E being due to the inability of a finite expansion being able to describe a step function with a substantial step size. Thus, for any finite N the CCC-calculated ionisation scattering amplitudes will generally not satisfy the symmetrisation postulate (23).

The analysis of Stelbovics (1999) shows that at $E/2$ the CCC-calculated amplitudes should be combined coherently. This is consistent with the step-function hypothesis and the $E/2$ amplitudes converging to half the step size, just like in Fourier expansions. Accordingly, the unitarity preserving incoherent prescription given by Bray and Fursa (1996*a*) needs to be multiplied by 2, but only at $E/2$. Subsequently, the two combinations of amplitudes yield near identical results for all cases considered. This is due to the fact that the CCC amplitudes at $E/2$ satisfy the symmetrisation postulate, at least approximately. The effect of any deviation from this on the TDCS is particularly small, see the discussion following (26). This reconciles the coherent versus incoherent combinations of the total-spin-dependent CCC amplitudes as both being effectively multiplications by 2. Recall that the CCC amplitude is already a coherent combination of its direct and exchange amplitudes depending on the total spin.

The above discussion is only applicable to the equal-energy-sharing kinematical region, where now we can claim to obtain from realistic calculations fully ab initio results convergent in both shape and magnitude. The situation for the asymmetric kinematical region is much less satisfactory. We are still unable to obtain convergence generally at low-enough total energies E. The coherent amplitude combination of Stelbovics (1999) holds generally only if the CCC amplitudes in the region $[E/2, E]$ are identically zero. In other words, only if the step-function hypothesis is true then the ionisation amplitudes, to be used in comparison with experiment, may be unambiguously defined. In practice, for large enough E, when comparing with experiment the step-function idea is well-satisfied as we find that $|f_S^{(N)}(\boldsymbol{k}, \boldsymbol{q})| \gg |f_S^{(N)}(\boldsymbol{q}, \boldsymbol{k})|$ for $q < k$. Hence, a coherent or an incoherent combination makes no discernible difference from just using the amplitude $f_S^{(N)}(\boldsymbol{k}, \boldsymbol{q})$.

Comparison with experiment is somewhat mixed. We find it particularly disturbing that the fundamental e–H DDCS have not been accurately determined experimentally. We make this claim by reference to the inconsistency between the data of Shyn (1992) and Shah *et al.* (1987). Consistency between the present results and those of Berakdar and Klar (1993) further supports this claim. In our view it is more important to obtain accurate DDCS, preferably absolute, than performing more complicated TDCS experiments. In support of this we have given an extensive spin-resolved set of DDCS for future comparison.

Turning our attention to the TDCS we find the agreement with experiment somewhat inconsistent. At high energies the agreement is generally satisfactory. This varies, sometimes quite substantially, as the incident energy is reduced. We believe that the CCC results presented accurately reflect the close-coupling approach to ionisation in that further even larger calculations, when computer resources permit, will not yield substantially different results. There is some uncertainty associated with the semi-empirical rescaling of the cross sections for asymmetric energy-sharing kinematics. However, given the nature of some of the discrepancies, at this point, this is the least of our concerns. The fundamental question we have is whether or not the close-coupling approach to ionisation, as we have defined it, converges to the true TDCS. The result of the present study suggests that this is still an open question. Further measurements, particularly in order to eliminate the experimental inconsistencies presented, would be very welcome, and help answer this question.

While it is clear that the close-coupling formalism is unable to yield accurate SDCS for small enough E this does not necessarily affect the angular profiles of the TDCS as discussed earlier (Bray 1999). The equivalent-quadrature idea in application to the systematic generation of the square-integrable states helps to ensure rapid convergence in the angular profiles. This may be readily checked numerically, as we have here in Fig. 20 for $27{\cdot}2$ eV and did earlier at $15{\cdot}6$ eV (Bray 1999). The utility of the rescaling prescription depends on the accuracy of the estimate of the true spin-resolved SDCS. Should this become known, as appears likely (Baertschy *et al.* 1999), then more accurate rescaling may be performed than what was presented here. This, however, is only applicable to the asymmetric energy-sharing kinematics. At equal energy-sharing we are no-longer free to rescale our results as previously thought.

The great strength of the close-coupling approach to ionisation is that it unifies the treatment of both the discrete and continuum parts of the atomic spectrum. We have already established the importance of treating the target continuum in application to discrete excitation processes (Bray 1994*b*). Similarly, we suspect that discrete excitation processes need to be treated in order to assure accuracy of ionisation calculations at all energies. We certainly hope that the present work will stimulate further e–H ionisation measurements and calculations, and therefore test the ability of the present implementation of the CCC theory to be predictive.

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