#### TOPICAL REVIEW

# Electrons and photons colliding with atoms

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Abstract. The immense progress that has occured during the 1990s in the field of electron—atom collision theory is discussed. We show how a solution of a small three-body model problem has led to an explosion of applications involving complicated real atomic collision systems. Consequently many fundamental electron-atom collision processes are considered as "solved", and accurate collision data of interest to science and industry have become available. However, we suggest that the present has only just seen the birth of modern atomic collision theory. There are many more important collision problems to be tackled, with guidence coming from experiment being as important as ever.

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## Contents

| 1             | Introduction  |                                     |                                      | 3    |
|---------------|---|-------------------------------------|--------------------------------------|------|
| 2             | Ele   | ctron-h                             | ydrogen scattering                   | 4    |
|               | 2.1 The Temkin-Poet or S-wave model                     |                                     |                                      | . 4  |
|               | 2.2   | 2.2 e-H discrete excitation         |                                      |      |
|               |   |                                     | nisation                             | 12   |
|               |   | 2.3.1                               | total ionisation cross sections      | . 12 |
|               |   | 2.3.2                               | singly differential cross section    | . 13 |
|               |   | 2.3.3                               | doubly differential cross sections   | . 14 |
|               |   | 2.3.4                               | fully differential cross sections    | . 14 |
| 3             | Photo- and related electron impact ionisation of helium |                                     |                                      | 16   |
|               | 3.1   | Two-el                              | ectron photoionisation               | . 17 |
|               |   | 3.1.1                               | Integrated cross sections            | . 17 |
|               |   | 3.1.2                               | Fully-differential cross sections    | . 18 |
|               | 3.2   | Electro                             | on-impact ionisation with excitation | . 19 |
|               | 3.3   | 3 Electron-impact double ionisation |                                      | . 20 |
| 4             | Electron-alkali atom scattering                         |                                     |                                      | 21   |
|               | 4.1 lithium   |                                     |                                      | . 22 |
|               | 4.2   | sodium                              | 1                                    | . 23 |
|               | 4.3   | potassi                             | ium                                  | . 23 |
| 5             | Electron-helium excitation and ionisation               |                                     |                                      | 25   |
|               | 5.1   | excitat                             | iion                                 | . 25 |
|               | 5.2   | ionisat                             | ion                                  | . 26 |
| 6             | Electron-alkaline-earths                                |                                     |                                      | 26   |
| 7 Conclusions |   |                                     | 31                                   |      |

#### 1. Introduction

The interest in the field of electron-atom collisions, and the closely related photon-atom interactions, ranges from fundamental science through to major industries. Interpretation of astrophysical plasmas relies critically on the knowledge of such collisions, particularly important presently due to the advancement in the ground- and space-based telescopes. Artificial plasmas, such as those occurring in fusion research or the lighting industry, also require knowledge of electron interactions with not only light but heavy atomic and ionic targets. Often a collision system that appears to have only scientific interest may be of assistance in dealing with problems of interest in industrial applications. For example, a theory that is able to accurately treat electron-impact double ionisation, often labelled as (e,3e), is likely to yield accurate results for doubly excited bound states of targets such as Ba, of importance to the lighting industry.

Solving electron-atom collision problems poses both formal and computational difficulties. At the base we have the fundamental Coulomb three-body problem of electron-atomic hydrogen collisions that only recently has been claimed to be solved (Rescigno et al 1999). The primary complexity arises from the difficulties associated with treating three or more particles in the continuum interacting out to infinite distances via the Coulomb potential. To date most of the progress has come from theories which are designed to avoid this boundary condition problem, but concentrate on the inner region instead. Theories which explicitly take into account the boundary conditions have thus far found it difficult to treat the inner region with the same accuracy, but much research in this direction is still ongoing.

We hope the review will serve a number of purposes. For the experimentalists and theorists in the area we give our perspective as to what problems are solved and which remain and are most urgent. For the more general reader and students entering the area, in addition to the above, we give an evolutionary perspective. Given the modern-day pressures to produce applicable research, we feel the example of how this happens following a fundamental model study without applications in mind, will be a valuable one.

The field of electron-atom computation was arguably began by Massey and Mohr (1932), and works around that period. Essential formulation for multi-channel scattering was presented that is still in use today. Due to computational constraints approximations concentrated on low and high incident energies, elastic scattering and excitation of just the lowest few excited states. Since that time progress has been steady with the major handicap being the available computational resources. The 1990s saw a rapid increase in the amount of computational memory available in readily affordable work-stations. To our mind this has been the dominant factor that is responsible for the progress we review here.

The structure of this work is as follows. We begin with a model electron-hydrogen problem which has been the testing ground for all successful approaches to the full electron-atom scattering systems. We then consider "one-electron" targets such as

atomic hydrogen and the alkalis, and then move on to helium and the "two-electron" targets that are the alkaline-earths. This is followed by what we think are the primary outstanding problems.

## 2. Electron-hydrogen scattering

#### 2.1. The Temkin-Poet or S-wave model

The full electron-hydrogen problem is complicated by the fact that the projectile electron moves in the three spacial dimensions. However, the shperical nature of the atom allows the reduction of these three dimensions to two, one angle and one spacial. The angular dimension may be expanded using Legendre polynomials in total orbital angular momentum  $L=0,\ldots,\infty$ . The difficulties associated with solving the relevant equations are much the same for each J, and so little generality is lost by considering only the L=0 case. The target electron motion may also be simplified to a single dimension without mush loss of generality. The resultant S-wave model problem was first considered by Temkin (1962) and then by Poet (1978) who gave some exact solutions for elastic and inelastic excitation transitions. The model corresponds to the full e-H scattering problem that retains only those target and projectile states of zero orbital angular momentum. Most importantly the problem retains the complexity associated with the treatment of ionisation and spin-dependence of the cross sections.

The value of this model has been recognised by all concerned with developing general electron-atom scattering theories. The field is far from static with new approaches still being developed and extended. Initially, time-independent closecoupling approaches were the first to be successfully applied to this model. They are based on the usage of negative- and positive-energy square-integrable pseudostates of the atom. Such approaches include the R-matrix method in its various forms (Burke and Robb 1975, Scholz et al 1991, Meyer et al 1995, Bartschat et al 1996, Gorczyca and Badnell 1997), Slater-based pseudostate methods (Oza and Callaway 1983, van Wyngaarden and Walters 1986), Laguerre-based pseudostate methods (Heller and Yamani 1974a, Bray and Stelbovics 1992b, Konovalov and McCarthy 1994), and references therein. Arguably, the greatest success has recently come from direct integration methods. The Exterior Complex Scaling (ECS) method was initially tested against the S-wave model (Baertschy et al 1999) and then spectacularly applied to the full problem (Rescigno et al 1999, Baertschy et al 2001). Another direct approach utilises the three-body boundary conditions, only known in partial-wave form for the S-wave model, to effectively obtain the total wavefunction, and has yielded the most accurate S-wave model solutions to date (Jones and Stelbovics 2000). In recent times various formulations of time dependent approaches have also shown considerable promise. (Ihra et al 1995, Pindzola and Schultz 1996, Pindzola and Robicheaux 1997, Madison et al 2000).

Thus far, the most widely used theory relies on the time-independent close-coupling

approach utilising pseudostates for the target continuum. To demonstrate this approach we use our own Laguerre-based pseudostate method known as the Convergent Close-Coupling (CCC) method (Bray and Stelbovics 1992a). The conclusions we draw are generally applicable to all such methods.

The detailed mathematical relations between the Laguerre based representations of the hydrogen continuum have been extensively studied in the 1970s (Heller and Yamani 1974b, Yamani and Reinhardt 1975, Broad 1978). Briefly, the continuum discretisation induces a quadrature rule for the integration over the true target continuum. In addition, the negative-energy states take into account the countably infinite set of true discrete eigenstates. Thus, the pseudostates do not truncate either the infinite discrete sum or the integral over the target continuum, but form a numerical approximation for both, which improves with increasing N.

The S-wave model is ideal for demonstrating how the close-coupling formalism works for both the discrete and the ionisation channels. There are three input parameters in the model, namely the Laguerre basis exponential fall-off parameter  $\lambda$ , the number of pseudostates  $n=1,\ldots,N$  of energy  $\epsilon_n^{(N)}$  and the total energy E of the system at which the calculation is to be performed. The close-coupling equations are then uniquely defined and upon solution lead to the  $i\to f$  transition matrix  $|T_{fi}^{(NS)}|^2$ , where S is the total spin. Supposing that  $E=\epsilon_n^{(N)}+k_n^2/2$  for  $n=1,\ldots,N_o$  (incident energy  $k_n^2/2>0$  in the open channels), then there are  $N_o^2$  output cross sections  $\sigma_{fi}^{(NS)}=|T_{fi}^{(NS)}|^2$  for each value of total spin S=0,1. Typically, we are only interested in scattering from the ground state (i=1) and only to the first few  $(f\leq 3)$  discrete states. In addition, the estimate of the total ionisation cross section obtained from summing the cross sections for excitation of the positive-energy states is of considerable interest. The key issue is that convergence to some acceptable accuracy be obtained for computationally realistic values of N.

In figure 1 two close-coupling calculations are given at a range of incident electron energies, one for N=10 and another for N=30. In both cases the paramater  $\lambda=2$ , which is optimal for the ground state. We see good convergence between the two calculations with the larger one showing fewer oscillations than the smaller. Both yield good agreement with the near-exact calculations of Poet (1978). Thus, the pseudoresonances, associated with relatively small basis sizes, can be simply thought of as indications of insufficiently large target-space quadratures in the close-coupling method. These results, first presented by Bray and Stelbovics (1992b), demonstrate the utility of the close-coupling approach and form the basis for the immense success of the close-coupling method throughout the 1990s.

Looking at figure 1 one may suspect that all aspects of the problem have been demonstrably solved. However, this is not the case. We are yet to examine the distribution, at a particular energy, of the ionisation cross section as a function of the energy of one of the outgoing electrons. Such distributions are known as the singly differential cross sections (SDCS). Integration over this secondary energy yields the total ionisation cross section (TICS) at a particular energy given in figure 1. For total energy

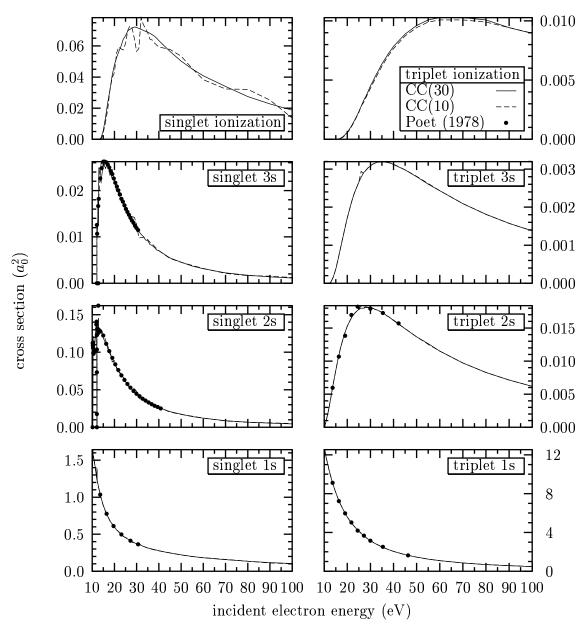


Figure 1. Cross sections (spin weights included) for excitation of the ground state of atomic hydrogen by electron impact in the s-wave model. The 30- and 10-state close-coupling calculations are due to Bray and Stelbovics (1992b). The solid dots are the near-exact results of Poet (1978)

E>0 the TICS  $(\sigma^{(SN)}_{\rm I})$  is defined from the relation for the total cross section for scattering from some initial state i

$$\sigma_{\text{Tot}}^{(SN)} = \sum_{f=1}^{N_o} \sigma_{fi}^{(SN)} \equiv \sum_{f:\epsilon_f^{(N)} < E} \sigma_{fi}^{(SN)}$$

$$= \sum_{f:\epsilon_f^{(N)} < 0} \sigma_{fi}^{(SN)} + \sum_{f:0 < \epsilon_f^{(N)} < E} \sigma_{fi}^{(SN)}$$

$$= \sigma_{\text{nb}}^{(SN)} + \sigma_{\text{I}}^{(SN)}, \qquad (1)$$

where  $\sigma_{\rm nb}^{(SN)}$  is the non-breakup cross section. The justification for such a separation is simple. The total cross section is the sum of the cross sections for excitation of all of the open channels. Since the negative-energy states converge to the true discrete eigenstates with increasing N it is clear that the summation of the excitation cross sections for the negative-energy states is an estimate of the total discrete excitation (non-breakup) cross section. The remainder must be the estimate of the total ionisation cross section.

Thus, the TICS is comprised from the excitation cross sections of the positive-energy pseudostates. Before examining these for a given total energy E it is interesting to study their behaviour as a function of E. This is what is given in figure 2. Here we have performed a 25-state calculation at many total energies E and plotted the excitation cross section for some selected positive-energy pseudostates as a function of  $E-\epsilon_n^{(25)}$ . The ninth state is the lowest positive-energy state whose energy is outside the given energy range. The other energies are indicated by arrows and correspond to the case where  $E=2\epsilon_n^{(25)}$ . The threshold for state n occurs when  $E=\epsilon_n^{(25)}$ .

There are a number of features of interest. We see that generally the cross sections start at zero, rise slowly initially, then rapidly to a maximum, and then diminish to zero again. The singlet cases show some oscillations whereas the triplet cases are quite smooth. In the latter case it appears that the cross sections remain particularly small until the total energy exceeds two times the threshold. Though less obvious for the singlet case, it is also seen that the rapid rise in the cross sections occurs after the total energy exceeds two times the threshold.

To illustrate things further let us now consider the SDCS at a particular energy. From (1) we may write

$$\sigma_{\rm I}^{(SN)} = \sum_{f:0 < \epsilon_f^{(N)} < E} \sigma_{fi}^{(SN)}$$

$$= \int_0^E de \frac{d\sigma}{de}^{(SN)}, \qquad (2)$$

where

$$\frac{d\sigma^{(SN)}}{de}(e_f) = \frac{1}{\sqrt{2e_f}} |\langle q_f^{(-)} | \phi_f^{(N)} \rangle|^2 \sigma_{fi}^{(SN)}, \tag{3}$$

and where  $q_f^{(-)}$  is the continuum eigenstate of energy  $q_f^2/2 = \epsilon_f^{(N)} = e_f$  (Bray and Fursa 1996a). The effect of the overlap in (3) is to change from the discrete to continuos normalization. However, this leaves the SDCS evaluated at only discrete energies  $\epsilon_f^{(N)}$  requiring some interpolation to define the SDCS at arbitrary e.

In figure 3 the results of three CCC(N) calculations are given for both the discrete excitation and ionisation at the total energy of E=3 Ry, which correspond to a projectile energy of 4 Ry or 54.4 eV. Turning to discrete excitation we see good convergence for the lowest-energy states for both spin channels, and the results may be compared to those given in figure 1. Note how the cross section for the least negative-energy state rises. This is not a deviation from the expected monotonically decreasing

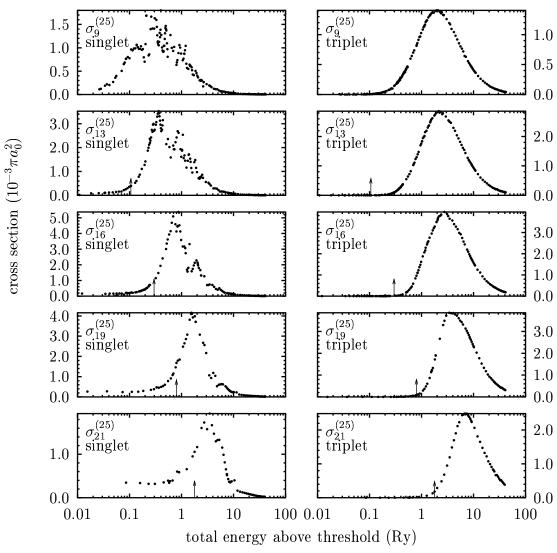


Figure 2. Singlet and triplet cross sections for excitation of the specified positive-energy states of the CCC(25) calculation of the S-wave model(Bray 1999). The arrows (when in energy range) indicate the energy  $\epsilon_n^{(25)}$  of the state at which point the total energy  $E=2\epsilon_n^{(25)}$ , see text.

sequence (expected to fall of as  $n^{-3}$ ), but an indication of how these states are taking into account the remaining infinite number of discrete states.

The ionisation SDCS is more interesting. Here we have very accurate results calculated by Jones and Stelbovics (2000) using a direct finite difference method (FDM). Since the two electrons are indistinguishable the SDCS is expected to be symmetric about E/2. However, the CCC results do not show such symmetry. For the triplet case they show good agreement with the FDM calculation in the energy range [0, E/2], but yield near-zero cross sections on the [E/2, E] interval. For the singlet case the situation is even worse. On the [0, E/2] interval the CCC results oscillate about the FDM ones, and are near zero on the [E/2, E] interval.

The behaviour of the CCC-calculated SDCS led to the suggestion that for infinite N

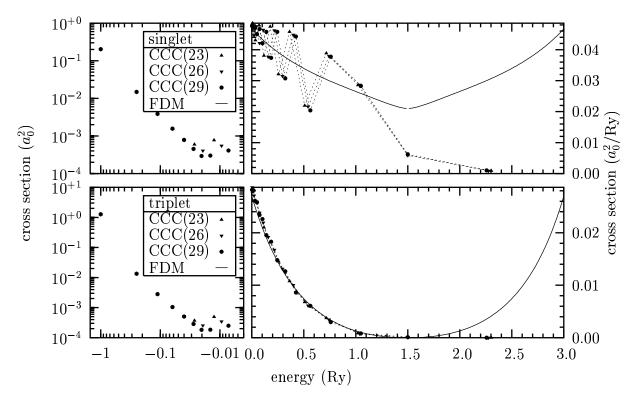


Figure 3. Singlet and triplet singly differential cross sections (SDCS) at a total energy E=3 Ry. The CCC calculations were performed using the indicated number of states, and in the singlet case the consecutive points have been connected with straight lines to guide the eye. The SDCS calculations of Jones and Stelbovics (2000) using a finite difference method are denoted by FDM.

the CCC-calculated SDCS would converge to a step function, with the SDCS being zero past E/2 (Bray 1997). For the triplet case the size of the step happens to be zero due to the SDCS being zero here by the Pauli Principle. We see that there is no difficulty with the finite expansions yielding the step function if the size of the step is zero. However, for the singlet case the SDCS at E/2 is non-zero, and we see considerable oscillations in the calculated SDCS. Even so, the integral of the singlet SDCS (or sum of excitation of the singlet cross sections for excitation of the positive-energy states) does converge, see figure 1. Stelbovics (1999) suggested that the CCC method behaves like a Fourier expansion of the underlying step-function amplitudes. The consequence of this is that at E/2 the amplitudes should converge to half their true size, and hence the SDCS to one quarter the true SDCS. If we compare the singlet CCC- and FDM-calculated SDCS we find a factor of approximately four difference. This conclusion also holds for the full e-H and e-He ionisation problems (Bray  $et\ al\ 2001$ ).

Thus, we see that the time-independent close-coupling method does not completely solve even the Coulomb three-body model problem considered here. However, it does solve for most aspects of the problem. All discrete transitions, including the total ionisation cross section, are accurately described. Fortunately, these are the most commonly required in applications. In addition, curiously, the ionisation problem with

equal energy outgoing electrons should‡ also be accurately described. If ionisation with asymmetric energy-sharing is much more probable than with symmetric energy-sharing, i.e. the size of the step is small, then all other ionisation processes may also be predicted accurately.

Before completing this section we should note that the most thorough test possible of the S-wave model is yet to be performed. Thus far theories have presented cross section data. It would be desirable to also present the complex phase of the discrete and ionisation amplitudes.

#### 2.2. e-H discrete excitation

Having demonstrated how the close-coupling method works for the S-wave model we now turn to full electron-hydrogen calculations and see how well the method works and its limitations. In the case of ionisation, we will be greatly assisted by the recent ECS calculation (Baertschy *et al* 2001) which appear to yield best overall agreement with available experiment.

The extra complexity of the full e-H scattering problem arises upon introduction of non-zero angular momentum to both the target and projectile space. Most of the details of various theories may be found in the preceding references. Here we shall concentrate on the major achievements of the close-coupling based approaches.

In the first instance the CCC method was developed in response to the long-standing discrepancy between two consistent experiments and all other theories for 2p excitation by 54.4 eV electrons. The experiments consisted of measuring the 54.4 - 10.2 = 44.2 eV outgoing electron in coincidence with the 2p photon on opposite sides of the scattering plane bisected by the incident beam. For each electron scattering angle the photon detector is moved over the accessible angular range. The coincidence counts were used to define the angular correlation parameters  $\lambda(\theta)$  and  $R(\theta)$ , where  $\theta$  is the electron scattering angle. These may be readily calculated theoretically, and have been shown to be related to the charge cloud distribution after collision (Andersen et al 1988).

In figure 4 the presently available experiments and some of the most reliable calculations are presented. Prior to the development of the CCC theory in the early 1990s there were substantial discrepancies at the backward angles between the best available IERM (Scholz et al 1991) and PSCC (van Wyngaarden and Walters 1986) theories and the two experiments performed in the early 1980s. The theories generally agreed with each other as did the two sets of measurements. This suggested that the measurements invalidated the existing theories, and hence motivated us to develop the most accurate one to date. To our great disappointment at the time the CCC theory yielded results much in agreement with the previous theories and so arguably also invalidated by experiment. However, subsequent angular correlation measurements by Yalim et al (1997) are in complete support of the theories. The most recent measurements of O'Neill et al (1998) are in between the old measurements and the \$\frac{1}{2}\$ We, as yet, are unable to explain why this appears not to be so for the full e-H problem(Bray 2000b)

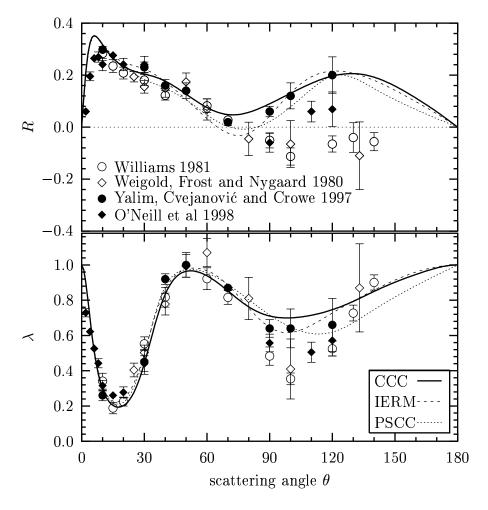
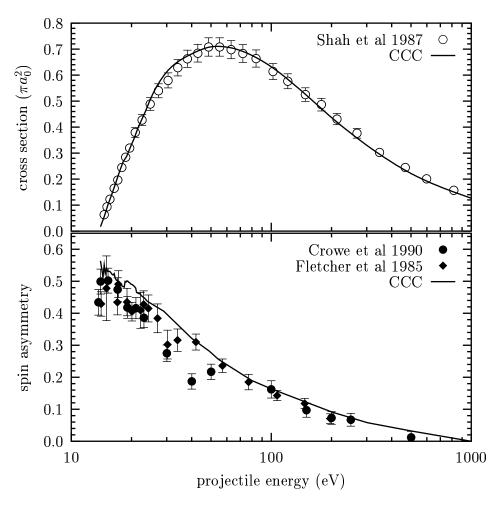


Figure 4. Angular correlation parameters  $\lambda$  and R for 2p excitation of atomic hydrogen by 54.4 eV electrons. The measurements are due to Williams (1981), Weigold et al (1980), Yalim et al (1997), and O'Neill et al (1998). The Intermediate Energy R-matrix (IERM) calculations are due to Scholz et al (1991), the Pseudostate Close-Coupling (PSCC) calculations are due to van Wyngaarden and Walters (1986), and the CCC calculations are due to Bray and Stelbovics (1992a).

theories. They use a more complicated technique, where the polarization of the photon is measured to yield the closely related Stokes parameters. Thus, the experimental situation is much less clear than previously thought, and it can no longer be claimed that the early 80s measurements invalidate the theory.

It is our view that the close-coupling theory will yield accurate electron-hydrogen excitation amplitudes at all energies. Generally, attention has been moved to excitation of more complicated atoms. This view was very recently supported by the unprecedently accurate measurements of the e-H differential cross sections by Khakoo  $et\ al\ (1999)$  and found to be in excellent absolute agreement with the CCC theory.



**Figure 5.** Electron-impact total ionisation cross section and spin asymmetry. The measurements are due to Shah *et al* (1987) Crowe *et al* (1990) and Fletcher *et al* (1985). The CCC calculations are due to Bray and Stelbovics (1993).

#### 2.3. e-H ionisation

An area that is presently very active is that of electron-impact ionisation. Solution of the discrete excitation problem leaves ionisation as the last frontier. The goal now is to develop a complete scattering theory, one that yields accurate discrete and ionisation amplitudes for all incident energies.

The atomic hydrogen target is of particular importance due to its fundamental simplicity requiring no significant structure approximation. Unfortunately, experimentally it is more difficult to use than, for example, helium. Nevertheless there is a great body of relative, and some normalised, measurements of e-H ionisation from near threshold through to high energies.

2.3.1. total ionisation cross sections The ionisation measurements take a number of forms. The least detailed is the total ionisation cross section (TICS). This simply yields the probability of an ionisation event as a function of the projectile energy. The

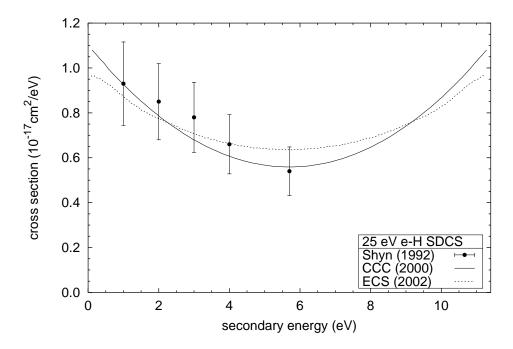


Figure 6. The singly differential cross section of atomic hydrogen upon 25 eV electron impact. The CCC calculations have target space states with  $l \leq 5$  and  $N_l = 18 - l$  states for each l (Bray 2000 a). The ECS curve is due to Baertschy (2002), and the experimental data are due to Shyn (1992).

associated spin asymmetry A is a measure of r the ratio of triplet to singlet TICS via A = (1-r)/(1+3r). The corresponding measurements and the CCC-calculated results are given in figure 5. Excellent agreement is found between the theory and experiments. While the CCC theory was the first fully ab initio theory to be able to reproduce these measurements, since that time a number of other close-coupling based theories have obtained similar results (Kato and Watanabe 1995, Bartschat and Bray 1996, Scott et al 1997).

2.3.2. singly differential cross section The next-most detailed ionisation process is the singly differential cross section (SDCS). This may be obtained from the integrated cross sections  $\sigma_{fi}^{(SN)}$  for the excitation of the positive-energy pseudostates via (3). While we may choose any of the energies given in figure 5, we take the case of 25 eV incident energy where there exists both experiment (Shyn 1992) and ECS theory (Isaacs et al 2001, Baertschy 2002).

In figure 6 the SDCS calculated using the CCC and ECS methods are compare with experiment. The raw CCC results are as oscillatory as those in figure 3. The presented smooth one curve is obtained upon assuming a quadratic form, with the two unknown parameters being determined from ab initio calculated TICS and the SDCS at the midpoint, see Bray (2000a) for details. We see that there is good agreement between the two theories and experiment, and so we can then move to the more detailed

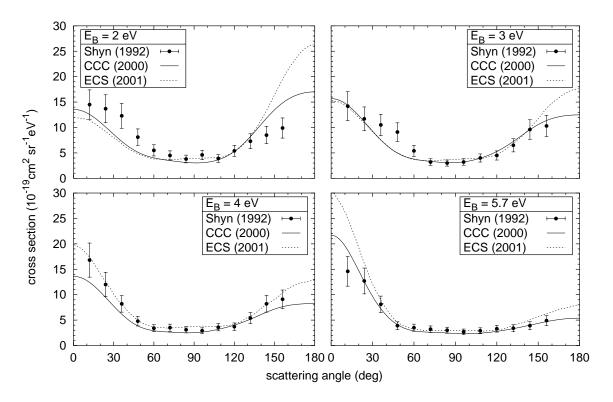


Figure 7. The doubly differential cross section of atomic hydrogen upon 25 eV electron impact. The CCC calculations have target space states with  $l \leq 5$  and  $N_l = 18 - l$  states for each l (Bray 2000a). The ECS curves are due to Isaacs  $et\ al\ (2001)$ , and the experimental data are due to Shyn (1992).

differential ionisation data.

2.3.3. doubly differential cross sections The probability of finding an outgoing electron of specified energy and scattering solid angle is determined by the doubly differential cross section (DDCS). Upon integration over the solid angle the SDCS is obtained. This is what was done by Shyn (1992) who measured the DDCS first.

Comparison of the two theories and experiment shows generally very good agreement. The biggest discrepancie between the theories are at the forward and backward angles, where there are no measurements and where the  $\sin(\theta)$  term in the angular integration reduces this discrepancy upon integration. Detailed, more accurate absolute DDCS measurements at even lower energies are presently underway (Khakoo 2002). These will help to distinguish between the ECS and the CCC theory, at least as far as the DDCS are concerned.

2.3.4. fully differential cross sections We next turn to the most detailed differential ionisation cross sections. These are often called fully or triply differential cross sections (TDCS), and give the angular distribution of say the faster outgoing electron given the energy and position of the slower electron. Upon integration over one of the solid angles

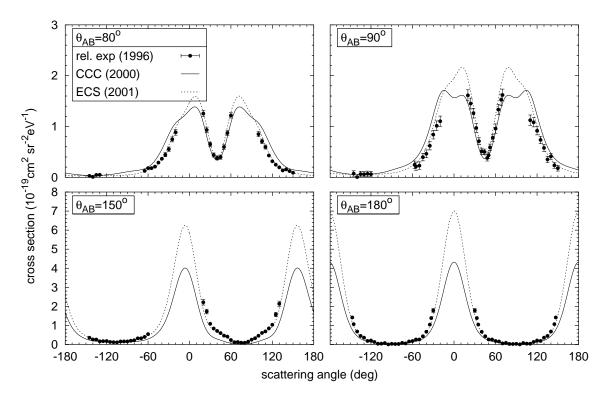


Figure 8. The coplanar equal energy-sharing triply differential cross sections for 25 eV electron-impact ionisation of the ground state of atomic hydrogen. The relative measurements are due to Röder *et al* (1996). The ECS and CCC calculations are due to Baertschy *et al* (2001) and Bray (2000b), respectively.

the corresponding DDCS is obtained.

There are a large number of possibilities to be considered. The TDCS depend on the excess energy E, the two energies of the outgoing electrons  $E_A + E_B = E$ , and the positions of the two detectors anywhere on a sphere. We will consider just the coplanar case with  $E_A = E_B = 5.7$  eV corresponding to  $E_0 = 25$  eV, for consistency with the DDCS and SDCS presented earlier. The special  $E_A = E_B$  case is interesting because the corresponding CCC amplitudes are obtained fully ab initio (Stelbovics 1999, Bray 2000b).

The TDCS for various geometries of the two coplanar detectors are given in figure 8. The data take the form of a surface as a function of position of the two detectors at  $\theta_A$  and  $\theta_B$ . For convenience experiment usually takes slices through the surface. The fixed  $\theta_{AB}$  geometries correspond to the case where the two detectors are moved together keeping their separation constant. The data are relative, but are internormalised requiring only a single scaling factor for the full set. We have chosen to normalise the experiment by best visual fit to the ECS calculations because this leads to best overall agreement with experiment. The CCC theory does not yield as good agreement with experiment as does the ECS theory. Surprisingly, the CCC theory appears to do best when the TDCS are smaller, which happens when the two electrons are closer together.

Yet, for the larger separations of the outgoing electrons the CCC theory substantially underestimates the TDCS. We do not understand why this problem occurs for the hydrogen target, particularly since it does not appear for the helium target discussed in what follows. Furthermore, a detailed study of asymmetric energy sharing (Bray 2000a) shows that generally the agreement with experiment is substantially improved, despite the fundamental problems depicted in figure 3, as compared to the symmetric energy sharing case. Until this issue is resolved we cannot claim to fully understand the close-coupling method.

Before we leave this section we would like to express the opinion that excitation of atomic hydrogen is basically a solved problem. A close-coupling based approach is capable of yielding accurate amplitudes for such cases. The S-wave model shows that direct application of the close-coupling method cannot fully solve even this simple problem, though with some external modification quite accurate results may be obtained. However, other methods, notably the ECS and FDM methods are able to do so. Furthermore, Rescigno et al (1999) claimed to be able to solve the full e-H three-body system. Thus far, the indications are that this may indeed be so. A more general application of the ECS approach to electron-atom collisions is most desirable.

## 3. Photo- and related electron impact ionisation of helium

Helium is a bound three-body system consisting of the nucleus and two electrons. Photoionisation is a collision process where a quantum of electromagnetic energy is absorbed by the helium atom and one of the atomic electrons is ejected in the continuum. There has been much progress in this field in recent times. We invite the interested reader to obtain the recent Topical Review by Briggs and Schmidt (2000) on the subject. Here we concentrate on the natural evolution from calculations of the e-H system to those considered here.

At most practical photon energies the electromagnetic field can couple to only one electron. Changing the quantum state of the second electron can take place either via electron-electron interaction in the bound state of the He atom or electron scattering of the first ejected electron on the residual He<sup>+</sup> ion. Electron-electron interaction in a bound state of He can be described with a high accuracy by employing a sufficiently large Hylleraas or multi-configuration Hartree-Fock expansion. Electron scattering on the He<sup>+</sup> ion is very similar to that of e-H scattering as the wave functions for He<sup>+</sup> belong to the same family as those of atomic hydrogen, except with Z=2. Another minor difference is that the target has an asymptotic charge requiring the use of Coulomb waves (including bound states) for the description of the projectile rather than plane waves. These are relatively simple modifications, and the first application of the CCC method to e-He<sup>+</sup> scattering was able to quantitatively describe the total ionisation cross section (Bray et al 1993), as was the case for the e-H system earlier (Bray and Stelbovics 1993).

#### 3.1. Two-electron photoionisation

Two-electron photoionisation is a special case of photoionisation where absorption of a single photon changes quantum states of both atomic electrons either by promoting the second electron to an excited state (excitation and photoionisation - EPI) or ejecting it in to the continuum (double photoionisation - DPI).

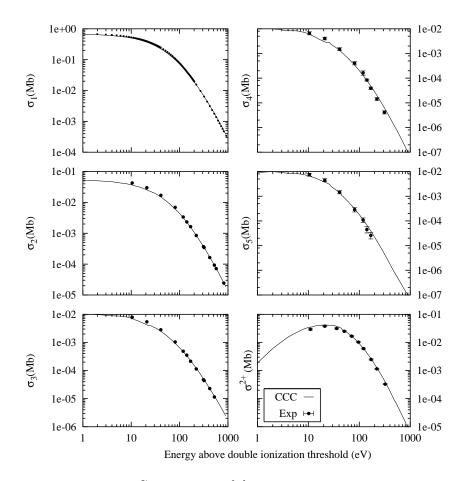


Figure 9. Cross-sections of the ground state photoionisation  $\sigma_1$ , photoionisation with excitation  $\sigma_n$  to  $n=2\ldots 5$  ion states and double photoionisation  $\sigma^{2+}$  in He. The solid line is the CCC calculation by Kheifets and Bray (1998*d*). The experimental data for ground state ionisation are by Samson *et al* (1994), ionisation-excitation by Wehlitz *et al* (1997), and for the double photoionisation by Dörner *et al* (1996)

3.1.1. Integrated cross sections The above-mentioned success suggested that the theory was able to describe two-electron transitions induced by a photon in the presence of the He nucleus. This encouraged Kheifets and Bray (1996) to apply the CCC method to EPI and DPI of helium. Extra work was required to obtain an accurate ground state of helium and evaluation of the dipole matrix elements, see also Kheifets and Bray (1998c). The results were very encouraging. In figure 9 the integrated cross sections are presented for the EPI and DPI processes. Agreement with experiment is excellent over a wide range of photon energies and a large variation of the cross-sections.

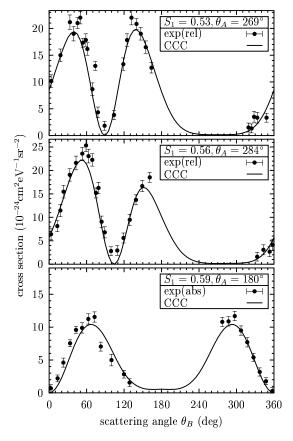


Figure 10. Triply differential cross sections for double photoionisation of the ground state of helium with 10 eV outgoing electrons. The  $\theta_A=180^\circ$  measurement is absolute (Schwarzkopf and Schmidt 1995, Schwarzkopf and Schmidt 1996), others are all relative (Schwarzkopf et al 1993), and have been normalized by best visual fit to the calculation (Kheifets and Bray 1998b).

3.1.2. Fully-differential cross sections Such good agreement with the integrated cross sections invited inspection of the fully differential cross sections. In figure 10 we give the TDCS for the case of 99 eV linearly polarised photons, of given Stokes parameter  $S_1$ , leading to ejection of two 10 eV electrons. Note that the double ionisation threshold is 24.6 + 54.4 = 79 eV. We see excellent agreement of the CCC calculation (Kheifets and Bray 1998b) with experiment. We believe that the double photoionisation problem of helium with equal-energy outgoing electrons is effectively solved at all energies (Kheifets and Bray 2000), using just the close-coupling approach. Note how this is in contrast to our experience with the corresponding e-H case.

Furthermore, the case of asymmetric energy sharing has caused few difficulties. The same problems as presented in figure 3 occur here also. Nevertheless, reasonably accurate predictive results are able to be obtained. For example, the initially presented experimental data (Mergel et al 1998) did not agree, in shape or magnitude, with the predictions of the CCC theory (Kheifets and Bray 1998a). However, subsequent remeasurement showed excellent agreement with the CCC predictions (Achler et al 2001).

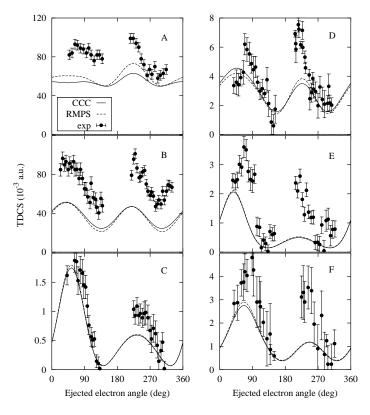


Figure 11. In-plane angular distribution of the ejected electron for ionisation-excitation to the He<sup>+</sup> n=2 states. The experimental results of Dupré et al (1992) are shown on the left at the ejected electron energies of 5 eV (A), 10 eV (B) and 75 eV (C). The experimental results of Avaldi et al (1998) are shown on the right at ejected electron energies of 10 eV (D), 40 eV (E) and 20 eV (F). The experimental data are compared with the CCC and RMPS calculations by Kheifets, Bray and Bartschat (1999).

#### 3.2. Electron-impact ionisation with excitation

Atomic ionisation by a fast particle impact can be treated within a formalism which is very similar to that for photoionisation. If the energy of the projectile is much larger than that of the ejected electron the interaction of the projectile with the target can be treated perturbatively by employing the Born series. The first term in this series (the first Born approximation - FBA) is sufficient to describe a two-electron transition in the helium atom either via the ground state correlation or the inelastic e-He<sup>+</sup> scattering. The FBA model then can be solved by employing a correlated ground state wave function and applying the same close-coupling formalism as for the single-photon two-electron transitions (EPI and DPI processes) (Kheifets et al 1994). The only difference with photoionisation is that in addition to the dipole scattering channel all other angular momenta contribute to the ionisation amplitude.

The FBA model for the electron-impact ionisation of He with simultaneous excitation has been attempted in different computational schemes. In addition to the CCC calculations, the R-matrix method with pseudo-states (RMPS) was employed by

Kheifets, Bray and Bartschat (1999). Both methods produced very similar results (see figure 11) but were quite different from close-coupling calculations of Marchalant et al (1998). The latter close-coupling model was revised and its results were subsequently found to be in perfect agreement with the CCC and RMPS predictions (Marchalant et al 1999). The need for higher order terms has been demonstrated (Marchalant et al 1999, Fang and Bartschat 2001), which becomes greater as the incident electron energy is reduced.

We suggest that this field is in its infancy. It is a true four-body Coulomb problem, and is a prototype of a large class of problems such as electron scattering on group II elements. Electron impact two-electron excitation is important in applications involving such elements where, unlike in helium, there are doubly excited bound states.

#### 3.3. Electron-impact double ionisation

Double ionisation of the helium atom by electron impact (e,3e-reaction) follows naturally from the above. Instead of taking the amplitudes for discrete excitation of He<sup>+</sup>, the positive-energy states are used to define the required amplitudes, just like in double photoionisation. Most of existing experimental data were obtained in a highly asymmetric kinematics where a very fast (few keV) projectile knocks out a couple of slow (few eV to few tens of eV) electrons. In this case the FBA formalism is adequate to describe the projectile-target interaction whereas the interaction of the two slow ejected electrons should be treated non-perturbatively.

The first (e,3e) experiment of the Orsay group performed at a very high incident energy of 5.5 keV and a small momentum transfer  $q \ll 1$  (Taouil et al 1998) was described qualitatively by the FBA-CCC model (Kheifets, Bray, Duguet, Lahmam-Bennani and Taouil 1999) and by the Coulomb four-body final state (C4FS) method (Lahmam-Bennani et al 1999). Recently, the Orsay group performed the experiment at an incident energy of 1 keV (Lahmam-Bennani et al 2001). These results were compared with different FBA calculations based on the three-body Coulomb waves method (known in the literature as BBK), C4FS and CCC methods. Considerable deviations between theory and experiment were observed and assigned to contributions of scattering processes whose description goes beyond the FBA. This explanation seems plausible in view of a relatively low energy of the incident electron. On the other hand, results of the Freiburg experiments at an incident energy of 2 keV, both in the low-qregime (Dorn et al 2001) and the impulsive regime q > 1 (Dorn et al 2002), were found in a generally good agreement with the FBA-CCC calculations. The theory explained well the main features of the experimental fully resolved five-fold differential cross-section (FDCS). Only minor deviations of the experiment from the symmetry expected in the FBA regime were not reproduced by the FBA-CCC theory.

Clearly, incident electron energy in (e,3e) reactions can always be taken sufficiently low so that there is a need for higher Born corrections. However, at this stage, even FBA calculations from different models strongly disagree. This could be seen in figure 12

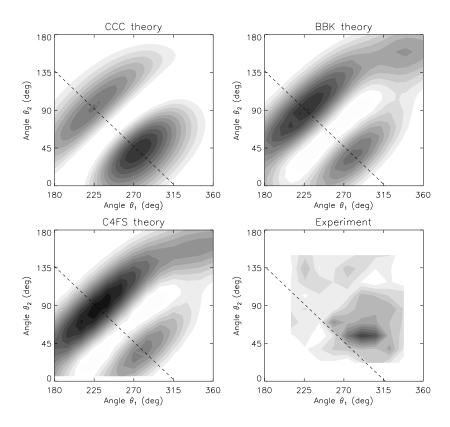


Figure 12. Contour plots of the (e,3e) FDCS at the kinematical conditions of the experiment by Lahmam-Bennani et al (2001). The escape angles of the two slow ejected electrons  $\theta_1$  and  $\theta_2$  are shown on the axes. Only the quadrant of the experimentally accessible range of angles is displayed. Top left - CCC calculation, top right - 3C calculation, bottom left - C4FS calculation, bottom right - experiment. The dashed line indicates the symmetry axis of the FBA model.

where the 3C and C4FS calculations, while very close to each other, are far apart from the CCC calculation. In contrast, similar  $(\gamma,2e)$  calculations performed with the 3C and CCC models produce very close, if not identical, results (Cvejanović *et al* 2000, Dawson *et al* 2001, Bolognesi *et al* 2001).

Intensive work is now underway to include higher Born corrections into theoretical models of the (e,3e) reaction (Berakdar 2000). However, before this is attempted, convergent FBA results have to be determined, similar to the case discussed in subsection 3.2.

## 4. Electron-alkali atom scattering

Soon after the development of the CCC theory for e-H scattering (Bray and Stelbovics 1992a) the technique was generalised to incorporate alkali metal targets (Bray 1994b). This was done by reducing these atoms to a quasi one-electron system. The valence electron was assumed to be moving under the influence of the frozen-core Hartree-Fock potential. In addition, for the heavier alkalis a phenomenological core-polarization

potential was added. The resulting change to the e-H formalism was a replacement of the nucleon potential (-1/r) by a non-local potential which had the same asymptotic behaviour. Such approximations may be readily tested by examining the structure of the derived atomic discrete states, and have been found to be very satisfactory.

Primary motivation for extending the code to the alkali targets was that at the time comparison with e-H experiment was unsatisfactory, see figure 4, and we hoped that application to the alkalis would shed some light on the problem. Alkalis have a big advantage over atomic hydrogen from the experimental perspective. Target preparation is a lot easier, and highly accurate superelastic techniques, where the atom is prepared in an excited state by a laser of suitable energy and deexcitation upon electron impact is measured, are able to be performed.

## 4.1. lithium

We begin by looking at the simplest of the alkalis, namely lithium. In figure 13 we present the spin-averaged Stokes parameters  $P_n$  and the derived charge cloud orientation

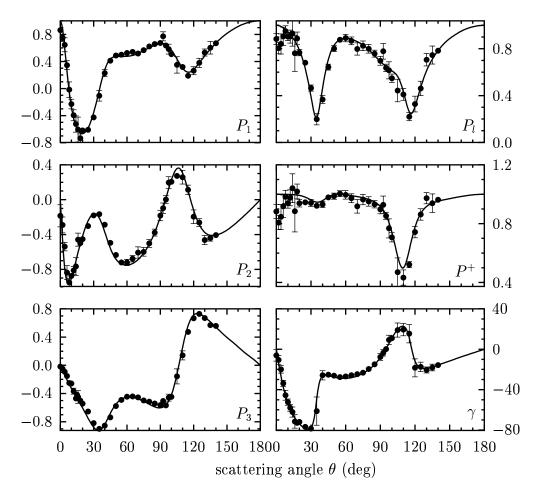
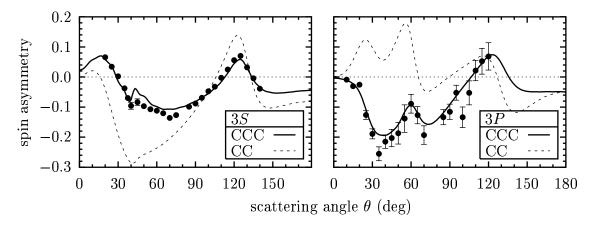


Figure 13. Stokes parameters  $P_n$  and derived orientation parameters for the lithium 2P excitation by 7 eV electrons. The data and CCC theory are from Karaganov *et al* (1998).



**Figure 14.** Spin asymmetries for elastic scattering and 3P excitation of the ground state of sodium by 20 eV electrons. The CCC calculations treat the full target spectrum, wherea as those denoted by CC treat only the sodium discrete spectrum (Bray 1994b). The experimental data were reported by Kelley *et al* (1992).

parameters for 7 eV electron impact excitation of the 2P state of lithium. The highly accurate and detailed data effectively describe the 2P charge cloud as a function of the electron scattering angle. In this sense the information gained in such experiments is the same as those presented in figure 4, but we see the quality of the data is far superior, owing to the superelastic technique. The agreement between theory and experiment is complete.

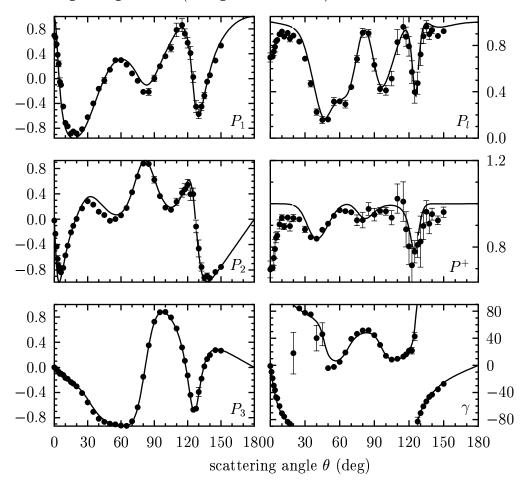
## 4.2. sodium

Historically, sodium was the first alkali to which the CCC theory was applied (Bray 1994b). The reason for this is that not only spin-averaged superelastic data was available (Scholten et al 1993, Sang et al 1994), but spin-resolved superelastically obtained data were also available (McClelland et al 1989, Scholten et al 1991) and references therein. This allowed for an unprecedently stringent test of the CCC, or any other, theory. For example, for a particular final state n such measurements yielded the ratio  $r_n$  of triplet to singlet differential cross sections, which is conveniently expressed as a spin asymmetry

$$A_n = \frac{1 - r_n}{1 = 3r_n}. (4)$$

In figure 14 we compare the calculated and measured spin asymmetries at 20 eV. Comparison is given not only with the CCC calculation, but also with a traditional close-coupling (CC) calculation which treates only the target discrete spectrum. We see excellent agreement between the CCC calculation and experiment, in marked contrast to the CC results. This was a most unexpected result that indicates just how difficult electron-atom calculations can be. Intuitively, one may have thought that the influence of the sodium continuum would be small on elastic scattering or the dominant 3P excitation. However, at some energies, as demonstrated here, this effect can be quite substantial. More complicated measurements and calculations involving excitation of

D-states also show good agreement (Shurgalin et al 1998).



**Figure 15.** Stokes parameters  $P_n$  and derived orientation parameters for the potassium 4P excitation by 10 eV electrons. The data and CCC theory are from Stockman *et al* (1998).

## 4.3. potassium

To test the CCC formulation for alkali targets further the Flinders group turned to the potassium target. In this case the target structure relies more heavily on phenomenological core polarization potentials. Furthermore, excitation and ionisation of core electrons becomes much more substantial, but as yet is unable to be treated by the CCC theory. The question is: how important are these considerations in describing the dominant 4P excitation channel. In figure 15 comparison between experiment and the CCC theory is given for the case of 4P excitation by 10 eV electrons. Once again, the accuracy of the data is only possible due to the usage of the superelastic technique. Agreement between theory and experiment is generally excellent, with a few exceptions. At the small scattering angles discrepancy disappears if the theory is convoluted with the experimental resolutions. Further study as a function of energy across the coreionisation thresholds did not reveal any major deviation between experiment and theory

(Stockman et al 2001).

This completes the brief overview of the quasi one-electron targets. We have seen that close-coupling theory describes scattering from such targets quite accurately, and so may be readily used to generate various integrated cross sections of practical interest.

Though we have barely touched on ionisation, owing to the fact that core-ionisation is not treated, for the lighter alkalis the direct ionisation process is dominant and should be accurately described. For example, initially the CCC theory predictions were at variance with the experimental predictions for e-Na total ionisation (Bray 1994a). However, subsequent measurements were found to be much closer to the theory than the earlier measurements (Johnston and Burrow 1995). We do note that Scott  $et\ al\ (2000)$  have shown how indirect ionisation processes can be included within the close-coupling formalism.

Lastly, application to heavy alkalis like Cs is showing some progress (Baum  $et\ al$  1999) and is presently an active area of investigation.

## 5. Electron-helium excitation and ionisation

#### 5.1. excitation

One of the more spectacular successes of the close-coupling (with pseudostates) theory has been observed after application to the helium target. Helium is an ideal target for the experimentalists and very detailed and accurate data exist over a large energy range. As such e-He data are often used as a standard allowing the determination of cross section data for other targets by reference to the helium data. Thus it is particularly important that theory and experiment agree well for this scattering system. Prior to the extension of the CCC theory to helium (Fursa and Bray 1995) this was not the case. Discrepancies, of the type seen earlier in e-H collisions (see figure 4) were commonplace.

For theorists, unlike experimentalists, it is the atomic hydrogen target that is ideal and not helium. However, fortunately, helium has no doubly excited discrete states, and so the frozen-core model, where one of the electrons is constrained to be in the 1s state of  $\mathrm{He^+}$ , leads to a sufficiently accurate structure. This has the effect of reducing the four-body problem to that of a three-body one. The field of e-He collisions is rather vast and recent progress covered in the Topical Review by Fursa and Bray (1997b). We use this work as our starting point.

As far as discrete excitation is concerned we only wish to make the following observation. While there is excellent agreement between theory and experiment for discrete excitation and total ionisation of the ground state, we are unaware of any resolution of the discrepancies for excitation from the metastable  $2^{1,3}$ S states (Fursa and Bray 1997b). The cross sections are very large and are crucially important to the understanding of any plasma containing He. This problem needs resolution urgently.

#### 5.2. ionisation

Ionisation of helium by electron impact is a field in itself. Owing to the ease with which the target may be delivered to the scattering centre the vast majority of experimental ionisation work has been done on this target. The CCC theory unifies the approach to excitation and ionisation processes in that both are calculated simultaneously. In fact Bray and Fursa (1996b) showed how a single CCC calculation at 100 eV was able to describe excitation to  $n \leq 3$  states, as well as singly, doubly, and triply differential ionisation cross sections. However, as discussed in section 2, at sufficiently low energies the CCC calculated SDCS develop unphysical oscillations. However, the CCC calculations yielded excellent agreement, but a factor of two too low, with the measurements of the TDCS in the case of outgoing electrons having the same energy, see Bray et al (1997) for example. This is now understood. The same considerations that applied to atomic hydrogen (Stelbovics 1999) apply to helium (Bray et al 2001). In particular, the raw CCC ionisation amplitudes converge to a step function, and are not meaningful when the energy of the pseudostate is greater than the corresponding plane wave. At the step, where the two energies are equal, the amplitude converges to half the required result, as in Fourier expansions of step-functions. Consequently, it was shown (Bray et al 2001) why the combination of amplitudes as suggested by Bray and Fursa (1996a) yielded results that are a factor of exactly two too low.

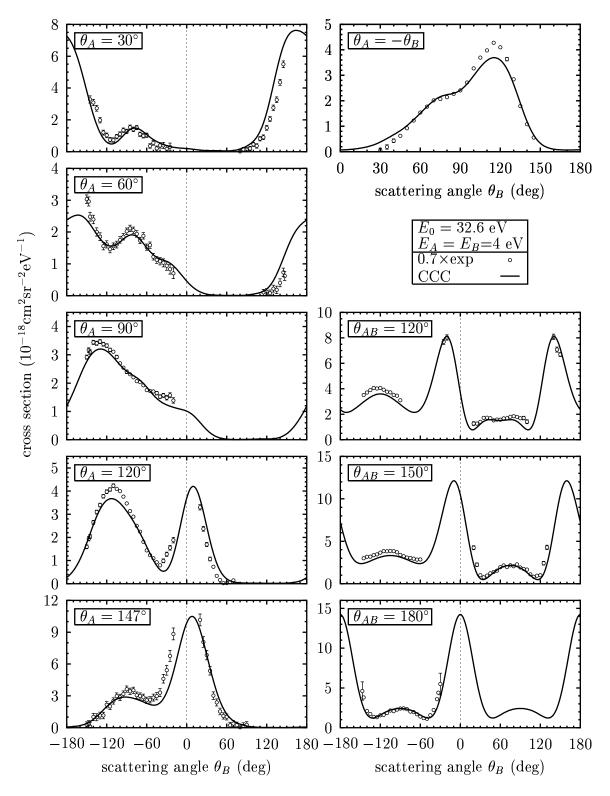
With this new information, thanks to Stelbovics (1999), we examine coplanar 32.6 eV e-He ionisation with two 4 eV outgoing electrons. The corresponding TDCS are given in figure 16. The details of the calculation and the experimental data have been given by Bray et al (1998).

We see excellent agreement between theory and experiment, though the magnitude of the latter has been reduced by 30%, which is a little outside the stated  $\pm 25\%$  experimental absolute value determination uncertainty. The agreement here is much superior to the case of atomic hydrogen with 5.7 eV outgoing electrons considered earlier in figure 8. Thus it appears that the CCC method works as expected for the more complicated He target than for H.

As far as asymmetric energy sharing is concerned the CCC method is still able to yield relatively accurate results, but external information is necessary at the lower energies. A detailed study of the e-He DDCS and TDCS with asymmetric energy sharing is presently underway.

#### 6. Electron-alkaline-earths

Extension of the CCC method to electron scattering from alkaline-earth atoms (Fursa and Bray 1997a) was the next natural step based on the work done for alkali atoms and helium. Alkaline-earth atoms (Be, Mg, Ca, Sr, Ba) can be accurately described as a quasy two-electron system: two active valence electrons above an innert core. Absence of inner core excitations in the discrete spectrum of the alkaline-earth atoms support



**Figure 16.** Coplanar triply differential cross sections in the indicated geometries for 32.6 eV electron-impact ionisation of the ground state of helium with two 4 eV outgoing electrons. The experimental data have been multiplied by 0.7 for best visual fit with the CCC theory. Calculations and the data were presented by Bray *et al* (1998).

this model. Whereas the frozen-core model is sufficient for helium, a substantially more complex configuration-interaction description has to be adopted here. Many discrete spectrum states have a large and often dominant contributions from two-electron excitations. Even a modest configuration interaction expansion results in a large number of states. The situation becomes even more complicated for heavy atoms (Sr, Ba) with relativistic corrections required. As yet it is impractical to account for all variety of one-and two-electron excitation and ionization processes. A typical calculation model for electron scattering from alkaline-earth atoms would neglect double ionization processes and most ionization with excitation channels.

In CCC calculations we first obtain a set of one-electron orbitals by diagonalization of Hamiltonian for the singly charged ion, in a Laguerre basis. This procedure is the same as calculation of target wave functions for alkali atoms. The basis sizes may be relatively large to obtain both the low- and high-lying descrete ionic eigenstates. We choose two-electron configurations in such a way that one of the electrons always occupies one of the low-lying ionic orbitals. This way we can model all doubly excited states in the discrete spectrum and the most important ionization with excitation channels.

For heavy alkaline-earth atoms (Sr, Ba) the nonrelativistic approximation fails. The most important relativistic effect is singlet-triplet mixing in the atomic wave functions. We model this effect (Zetner et al 1999) by calculating singlet-triplet mixing coefficients in the following way. First the one-body spin-orbit term of the Breit-Pauli Hamiltonian is diagonalised in the basis of the nonrelativistic wave functions. The semirelativistic scattering amplitudes can then be calculated as a sum over relevant nonrelativistic scattering amplitudes multiplied by corresponding singlet-triplet mixing coefficients.

Some transitions can be strongly affected by the singlet-triplet mixing. These are the transitions which can only occur via exchange scattering in the nonrelativistic calculation. They change substantially if the direct scattering becomes possible due to the singlet-triplet mixing. We will give an example of such a transition later in this section.

There is a large variety of scattering processes possible for electron scattering from alkaline-earth atoms with the resonance transition occupying a special place. It is the only transition for which very accurate experimental data are available, via the optical excitation function (Ehlers and Gallagher 1973, Leep and Gallagher 1976, Chen et al 1976, Chen and Gallagher 1976). Optical excitation function for a resonance  $nsns^1S - nsnp^1P$  transition in alkaline-earth atoms is a sum of direct excitation cross section and all cascades from high-lying levels to the  $nsnp^1P$  state.

In figure 17 we present comparison of experimental data with close-coupling calculations. Comparison of CCC with CC shows that even for the resonance transitions treating the target continuum is important. First order theoretical models which have been applied to these transitions, such as FOMBT and UDWA calculations (Clark et al 1989) or even fully relativistic DWA calculations (Srivastava, Zuo, McEachran and Stauffer 1992, Srivastava, McEachran and Stauffer 1992), are in substantially worse agreement with experiment.

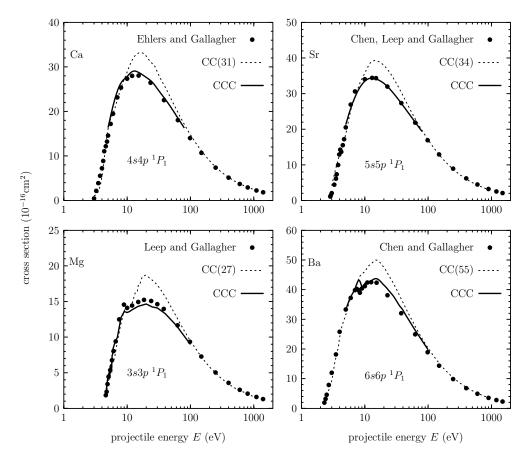


Figure 17. Optical excitation function for resonance transitions in Mg, Ca, Sr, and Ba. Experiments are due to Ehlers and Gallagher (1973), Leep and Gallagher (1976), Chen et al (1976), Chen and Gallagher (1976). The calculations labeled CC omit ionisation processes, those labeled CCC take ionisation into account. The Ba calculations were reported by Fursa and Bray (1999) and the Mg calculations by Fursa and Bray (1999). The others are in part discussed in Fursa and Bray (2002).

At particular energies of figure 17 detailed measurements of the shape of the charge cloud after excitation are available. We take just one example, presented in figure 18.

We see a generally good agreement between theories and the measured data. The general shapes are rather well reproduced. Consequently, it is our opinion that the resonance transitions do not provide as a sensitive test of theory as do other weaker transitions. A good example of such a transition is excitation of the  $5d^2$   $^3P_2$  level from the laser excited 6s6p  $^1P_1$  level of barium atom. The  $5d^2$   $^3P_2$  level is a doubly excited state which is strongly affected by configuration interaction. In addition, the nonrelativistic approximation fails for this level. Below we give major configurations for this level:

$$5d^{2} {}^{3}P_{2} : 0.745(5d^{2} {}^{3}P_{2}) - 0.427(5d6d {}^{3}P_{2}) + 0.363(6p^{2} {}^{3}P_{2})$$

$$+ 0.286(5d^{2} {}^{1}D_{2}) - 0.159(5d6d {}^{1}D_{2}) + 0.126(6p^{2} {}^{1}D_{2})$$

$$(5)$$

We present in Fig. 19 results of the CCC e-Ba calculation of DCS and EICP parameter  $L_{\perp}$  at 20 eV. It is fortunate that measurements for DCS and EICPs for this and many

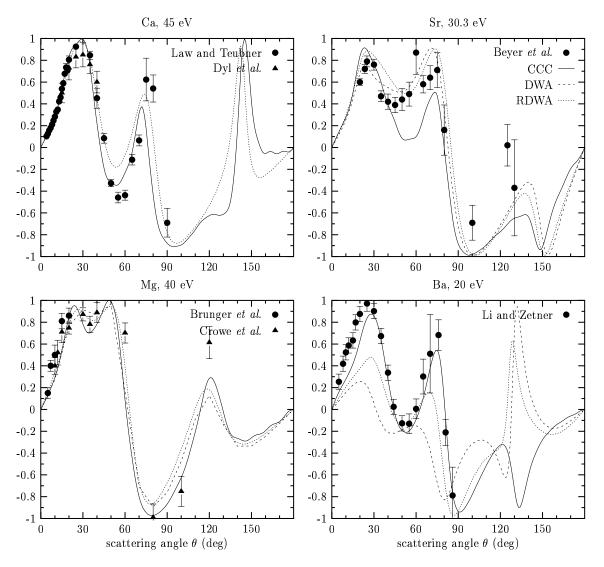
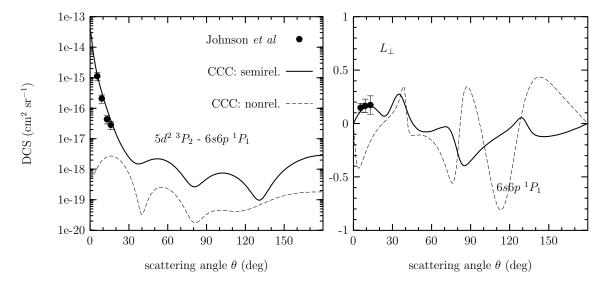


Figure 18. The resonance transition  $L_{\perp}$  parameter measured and calculated for the given atoms and incident electron energies. The experiments are dure to Brunger *et al* (1989), Law and Teubner (1995), Dyl *et al* (1999), Beyer *et al* (1994), Li and Zetner (1994) and Crowe *et al* (2002). Details of the theories may be found in Fursa and Bray (2002).

other excited-to-excited state transitions have been performed by Zetner et~al (Johnson et~al~2002, Johnson et~al~1999, Zetner et~al~1999, Zetner et~al~1997) at University of Manitoba. Fig. 19 demonstrate a very good agreement between experiment and our CCC results for both DCS and EICP parameter  $L_{\perp}$ . Note that in nonrelativistic approximation this would be an exchange only transition, the nonrelativistic CCC results for this transition are presented in Fig. 19. The strong forward peaking behaviour of the DCS is due to singlet-triplet mixing in the  $5d^2$   $^3P_2$  level. Small angle DCS is dominated by dipole-allowed transition between 6s6p  $^1P_1$  configuration and  $^1D_2$  configurations.

The integral cross section for the  $5d^2$   $^3P_2$ -6s6p  $^1P_1$  transition is dominated by



**Figure 19.** Differential cross section and parameter  $L_{\perp}$  for 20 eV electron excitation of the  $5d^2$   $^3P_2$  state from the 6s6p  $^1P_1$  of barium. Experiment is due to Johnson *et al* (2002)

forward scattering angles. Given good agreement of the semirelativistic CCC and experiment for differential cross section we have considerable degree of confidence in the integral cross sections calculated in the semirelativistic CCC method. Results for many other transitions have been recently published (Fursa et al 2002, Fursa et al 1999).

## 7. Conclusions

The above few examples demonstrate the power of the close-coupling method, of which CCC is just one implementation. While it has some inherent problems these are of minimal significance for real applications. The method works well from low to high energies, from excitation to ionisation. Nevertheless, the results above should be seen simply as "proof of principle". There is still immense amount of work ahead of us. The range of atomic and ionic targets thus far treated by the close-coupling method needs to increase to meet application demand. The incorporation of fully relativistic scattering theory is likely to be important at some stage. In addition, scattering theory for problems involving more than one centre, such as positron-atom scattering or ionatom collisions, is less developed.

Experiment has and will continue to play a central role in the development of theory. The more complicated the process the more important the experiment will be to guide theory. The importance of performing "complete" scattering experiments is well documented. These provide the most thorough test of the theoretically calculated scattering amplitudes.

We finish off with a wish-list for more experimental investigation:

- electron-impact excitation of the metastable states of helium,
- doubly differential cross sections for electron-impact ionisation of atomic hydrogen,

- double photoionisation of the alkaline-earths,
- spin-resolved experiments,
- electron scattering on the heavier alkalis and alkaline-earths, particularly at the larger scattering angles.
- and what ever else people wanna do.

#### Acknowledgments

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