

# The Electron–Atom Ionisation Problem\*

I. E. McCarthy

Electronic Structure of Materials Centre, Flinders University,  
GPO Box 2100, Adelaide, SA 5001, Australia.

## Abstract

Methods of calculating electron–atom ionisation as a three-body problem with Coulomb boundary conditions are considered. In the absence of a fully-valid computational method for a time-independent experiment the approximation is made that the incident electron experiences a screened potential. Approximations involving a final state that obeys the three-body Coulomb boundary condition are compared with the distorted-wave Born approximation and the convergent close-coupling method.

## 1. Introduction

There are several reasons for the interest generated by the electron–atom ionisation problem. The long-range Coulomb forces acting in all three two-body subsystems in the final state make its formulation a fascinating problem in mathematical physics (Chandler 1995). The diversity of kinematic regions that can be observed in experiments makes it possible to emphasise the interaction of different two-body subsystems.

From the point of view of calculating differential cross sections it is a good approximation to treat the problem as the interaction of two electrons with a positively-charged inert core, whose kinetic energy can be neglected without any essential simplification. The three-body electron–hydrogen problem has the two essential difficulties. These are the identity of the two electrons and the final-state charged three-body continuum.

We treat unsymmetrised ionisation amplitudes. Antisymmetry is achieved by means of exchange amplitudes obtained by relabelling the final-state electrons.

The momenta of electrons 1 and 2 in the final state are denoted by  $\mathbf{p}_1$ ,  $\mathbf{p}_2$ . The incident momentum is  $\mathbf{p}_0$ . The potentials between electrons 1 and 2 and the core are respectively  $v_1$  and  $v_2$ . The electron–electron potential is  $v_3$ . In all cases these potentials have the Coulomb form at long range. For hydrogen they are pure Coulomb forces. The kinetic energies of electrons 1 and 2 are  $K_1$ ,  $K_2$ . Electron 2 is bound initially in the state  $|\alpha\rangle$ .

The experimental kinematics is described for incident, fast and slow electrons, 0,  $f$  and  $s$  respectively. Kinetic energies are  $E_0$ ,  $E_f$ ,  $E_s$ , and momenta are  $\mathbf{p}_0$ ,

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$\mathbf{p}_f, \mathbf{p}_s$ . Polar angles relative to  $\mathbf{p}$  are  $\theta_f, \theta_s$ , and the relative azimuthal angle  $\phi$  is  $\pi - \phi_f + \phi_s$ . Common kinematic regions for experiments are as follows.

Coplanar asymmetric :  $\phi = 0, E_s \ll E_0, \theta_f$  small,  $\theta_s$  varied;

Coplanar symmetric :  $\phi = 0, E_s = E_f, \theta_s = \theta_f = \theta$  varied;

Noncoplanar symmetric :  $E_s = E_f, \theta_s = \theta_f = 45^\circ, \phi$  varied.

## 2. Formal Scattering Theory

Formal scattering theory (e.g. Gell-Mann and Goldberger 1953) treats the total stationary state of the system  $|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle$  in terms of the long-lifetime limit of wave packets arising from the time development of the channel state  $|\alpha\mathbf{p}_0\rangle$ . The total Hamiltonian is

$$H = K_1 + K_2 + v_1 + v_2 + v_3. \quad (1)$$

The entrance-channel Hamiltonian is

$$K = K_1 + K_2 + v_2. \quad (2)$$

The potential governing the scattering from one channel state to another is

$$V = H - K. \quad (3)$$

The entrance-channel state  $|\alpha\mathbf{p}_0\rangle$  describes a plane wave with momentum  $\mathbf{p}_0$  incident on a bound system with electron 2 in the state  $|\alpha\rangle$ . The potential in this channel is of short range so that the projectile is asymptotically a plane wave.

The time-reversed problem is equivalent. The total stationary state of the three-body system is  $|\Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2)\rangle$ . The asymptotic boundary condition describes three bodies with positive energy, interacting through Coulomb forces. In describing states we omit spin, which is a non-essential complication treated by antisymmetrisation at the end of the discussion. The asymptotic final state was first given by Rosenberg (1973), based on unpublished work by Redmond:

$$\langle \mathbf{r}_1 \mathbf{r}_2 | \Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2) \rangle \rightarrow (2\pi)^{-3} e^{i\mathbf{p}_1 \cdot \mathbf{r}_1} e^{i\mathbf{p}_2 \cdot \mathbf{r}_2} e^{i\Phi}. \quad (4)$$

The asymptotic phase  $\Phi$  is given in terms of the relative momentum  $\mathbf{p}_i$ , relative position  $\mathbf{r}_i$  and charge product  $z_i$  of each pair  $i = 1, 3$  by

$$\Phi = \sum_i \phi_i, \quad (5)$$

$$\phi_i = \eta_i \ln(p_i r_i + \mathbf{p}_i \cdot \mathbf{r}_i), \quad (6)$$

where  $\eta_i$  is the Sommerfeld parameter, equal to  $z_i/p_i$  in atomic units.

For computational purposes it is always useful to describe the projectile part of the channel state by a scattering state  $|\chi^{(\pm)}(\mathbf{p}_0)\rangle$  for a suitably-chosen local,

central, short-range potential  $U_1(r_1)$ . This potential is added to  $K$  and subtracted from  $V$ . The entrance-channel state becomes  $|\alpha\chi^{(+)}(\mathbf{p}_0)\rangle$ , which we call a distorted-wave channel state.

In the present distorted-wave problem, for bound states of electron 2, the potential governing the motion of electron 1 is

$$V - U_1 = v_1 + v_3 - U_1, \quad (7)$$

which is of short range.

For a short-range potential a time-independent experiment has an amplitude given in terms of stationary states by the  $T$ -matrix element:

$$\langle \mathbf{p}'_0 \beta | T | \alpha \mathbf{p}_0 \rangle = \langle \chi^{(-)}(\mathbf{p}'_0) \beta | V - U_1 | \Psi_\alpha^{(+)}(\mathbf{p}_0) \rangle, \quad (8)$$

where  $|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle$  is the solution of an integral equation, the Lippmann-Schwinger equation, whose driving term is the corresponding distorted-wave channel state:

$$|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle = |\alpha\chi^{(+)}(\mathbf{p}_0)\rangle + \frac{1}{E^{(+)} - K - U_1} (V - U_1) |\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle. \quad (9)$$

The essential question in formulating the ionisation problem is: can we define a short-range potential and a corresponding exit-channel state for the ionisation problem? If not, then we cannot define a Lippmann-Schwinger equation for the problem. A formal  $T$ -matrix element has been defined by Rosenberg (1973). The time-dependent state of three charged particles has been discussed by Dollard (1964), but no means of calculating the stationary state  $|\Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2)\rangle$  has been devised. Assuming this stationary state, the  $T$ -matrix element is given in terms of the entrance-channel state by applying time reversal to (8)

$$\langle \mathbf{p}_1 \mathbf{p}_2 | T | \alpha \mathbf{p}_0 \rangle = \langle \Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2) | V - U_1 | \alpha\chi^{(+)}(\mathbf{p}_0) \rangle. \quad (10)$$

Curran and Walters (1987) and Bray *et al.* (1994) have adopted the position that for very large  $r_1$  and finite  $r_2$  the potential  $V$  of (7) is of short range. The exit-channel Hamiltonian is then given by (2) and the exit-channel state is  $|\chi^{(-)}(\mathbf{p}_2)\chi^{(-)}(\mathbf{p}_1)\rangle$ , where  $|\chi^{(-)}(\mathbf{p}_2)\rangle$  is a time-reversed scattering state of the subsystem 2 and  $|\chi^{(-)}(\mathbf{p}_1)\rangle$  is a scattering state of  $U_1$ . The  $T$ -matrix element is

$$\langle \mathbf{p}_1 \mathbf{p}_2 | T | \alpha \mathbf{p}_0 \rangle = \langle \chi^{(-)}(\mathbf{p}_1) \chi^{(-)}(\mathbf{p}_2) | V - U_1 | \Psi_\alpha^{(+)}(\mathbf{p}_0) \rangle. \quad (11)$$

Adopting the same point of view Klar *et al.* (1993) reformulated the  $T$ -matrix element in terms of an auxiliary state  $|\Phi^{(-)}(\mathbf{p}_1, \mathbf{p}_2)\rangle$ :

$$\begin{aligned} \langle \mathbf{p}_1 \mathbf{p}_2 | T | \alpha \mathbf{p}_0 \rangle &= \langle \Phi^{(-)}(\mathbf{p}_1, \mathbf{p}_2) | \bar{H} - E | \Psi_\alpha^{(+)}(\mathbf{p}_0) - \alpha\chi^{(+)}(\mathbf{p}_0) \rangle \\ &+ \langle \Phi^{(-)}(\mathbf{p}_1, \mathbf{p}_2) | V - U_1 | \alpha\chi^{(+)}(\mathbf{p}_0) \rangle. \end{aligned} \quad (12)$$

Here the Hamiltonian in the first term operates on the bra vector. The first term of (12) may be considered as a correction to the second term, which may be minimised by an optimum choice of either, or preferably both, of two criteria:

1.  $U_1$  should be chosen so that  $|\alpha\chi^{(+)}(\mathbf{p}_0)\rangle$  is a good approximation to  $|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle$ .
2.  $|\Phi^{(-)}(\mathbf{p}_1, \mathbf{p}_2)\rangle$  should approximate  $|\Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2)\rangle$  closely.

Note that (12) becomes (10) if criterion 2 is exactly fulfilled. Note also that the coordinate representation of the ket vector in the first amplitude of (12) vanishes asymptotically. Therefore it is sufficient to satisfy the initial-state boundary condition. For a short-range potential  $V$  it is not necessary to satisfy the final-state boundary condition to make the first amplitude converge.

### 3. Choice of the Distorting Potential

The distorting potential  $U_1$  is chosen so that  $|\alpha\chi^{(+)}(\mathbf{p}_0)\rangle$  is as close as possible to the exact three-body state  $|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle$ . We project the integral equation (9) onto the initial bound state  $|\alpha\rangle$ , and expand in the complete set  $|\mu\rangle$  of target states:

$$\begin{aligned} \langle\alpha|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle &= |\chi^{(+)}(\mathbf{p}_0)\rangle + \sum_\mu \langle\alpha| \frac{1}{E^{(+)} - (K_1 + U_1) - (K_2 + v_2)} |\mu\rangle \\ &\times \langle\mu|V - U_1|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle. \end{aligned} \quad (13)$$

The approximation requires the second term of (13) to be small. Making the approximation, the second term becomes

$$\frac{1}{E^{(+)} - (K_1 + U_1) - \epsilon_\alpha} \langle\alpha|V - U_1|\alpha\rangle |\chi^{(+)}(\mathbf{p}_0)\rangle. \quad (14)$$

The approximation is consistent if (14) vanishes, requiring

$$U_1 = \langle\alpha|V|\alpha\rangle. \quad (15)$$

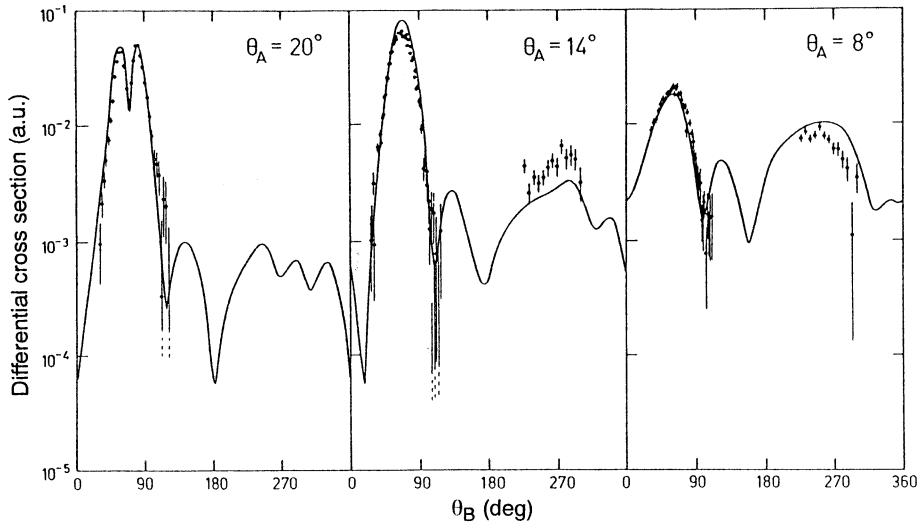
The optimum choice of  $U_1$  is the average of  $V$  for the initial bound state  $|\alpha\rangle$  of electron 2.

### 4. The Distorted-wave Born Approximation

The distorted-wave Born approximation (DWBA) is most-easily understood as the replacement of  $|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle$  in (11) by the optimum distorted-wave channel state, chosen according to (15). Potentials that are independent of  $\mathbf{r}_2$  vanish because of the orthogonality of the eigenstates of  $K_2 + v_2$ . The approximation is

$$\langle\mathbf{p}_1\mathbf{p}_2|T|\alpha\mathbf{p}_0\rangle = \langle\chi^{(-)}(\mathbf{p}_1)\chi^{(-)}(\mathbf{p}_2)|v_3|\alpha\chi^{(+)}(\mathbf{p}_0)\rangle. \quad (16)$$

We emphasise that it is not a first-order approximation but a weak-coupling approximation for  $|\Psi_\alpha^{(+)}(\mathbf{p}_0)\rangle$ , justified by the considerations of Section 3. This approximation has set the standard for calculations of (e,2e) differential cross sections. It is excellent at high energy, as shown in Fig. 1 for coplanar asymmetric ionisation from the 3p orbital of argon at  $E_0 = 1000$  eV.



**Fig. 1.** Coplanar asymmetric ionisation from the 3p orbital of argon at  $E_0 = 1000$  eV,  $E_s = 120$  eV (Avaldi *et al.* 1989).

### 5. The Approximation of Brauner, Briggs and Klar

The BBK approximation (Brauner, Briggs and Klar 1989) replaces the exact state  $|\Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2)\rangle$  in (10) by the product of two distorted waves with Coulomb boundary conditions and a correlation factor  $C(\mathbf{p}_1 - \mathbf{p}_2)$ , whose coordinate-space representation is

$$C(\eta, \mathbf{k}, \mathbf{r}) = \Gamma(1 - i\eta) e^{-\pi\eta/2} F_{11}(i\eta; -i(kr + \mathbf{k} \cdot \mathbf{r})), \quad (17)$$

where

$$\eta = 1/2k, \quad \mathbf{k} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2), \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2. \quad (18)$$

The correlated motion of electrons 1 and 2 in the final state is represented by a repulsive Coulomb wave. The approximation is

$$\langle \mathbf{p}_1 \mathbf{p}_2 | T | \alpha \mathbf{p}_0 \rangle = \langle \bar{\chi}^{(-)}(\mathbf{p}_1) \chi^{(-)}(\mathbf{p}_2) C(\mathbf{p}_1 - \mathbf{p}_2) | V - U_1 | \alpha \chi^{(+)}(\mathbf{p}_0) \rangle. \quad (19)$$

The original BBK calculation was for hydrogen with  $U_1 = 0$ . We have generalised it for larger targets. In (19),  $|\bar{\chi}^{(-)}(\mathbf{p}_1)\rangle$  is distinguished from  $|\chi^{(-)}(\mathbf{p}_1)\rangle$  by the Coulomb boundary condition for the former, and the plane-wave boundary condition for the latter. Note that the BBK approximation satisfies the three-body final-state boundary condition (4).

### 6. Coplanar Symmetric Ionisation of Helium

For small  $\theta$ , coplanar symmetric ionisation emphasises the effect of the electron-electron correlation in the final state. This is not explicit in the DWBA,

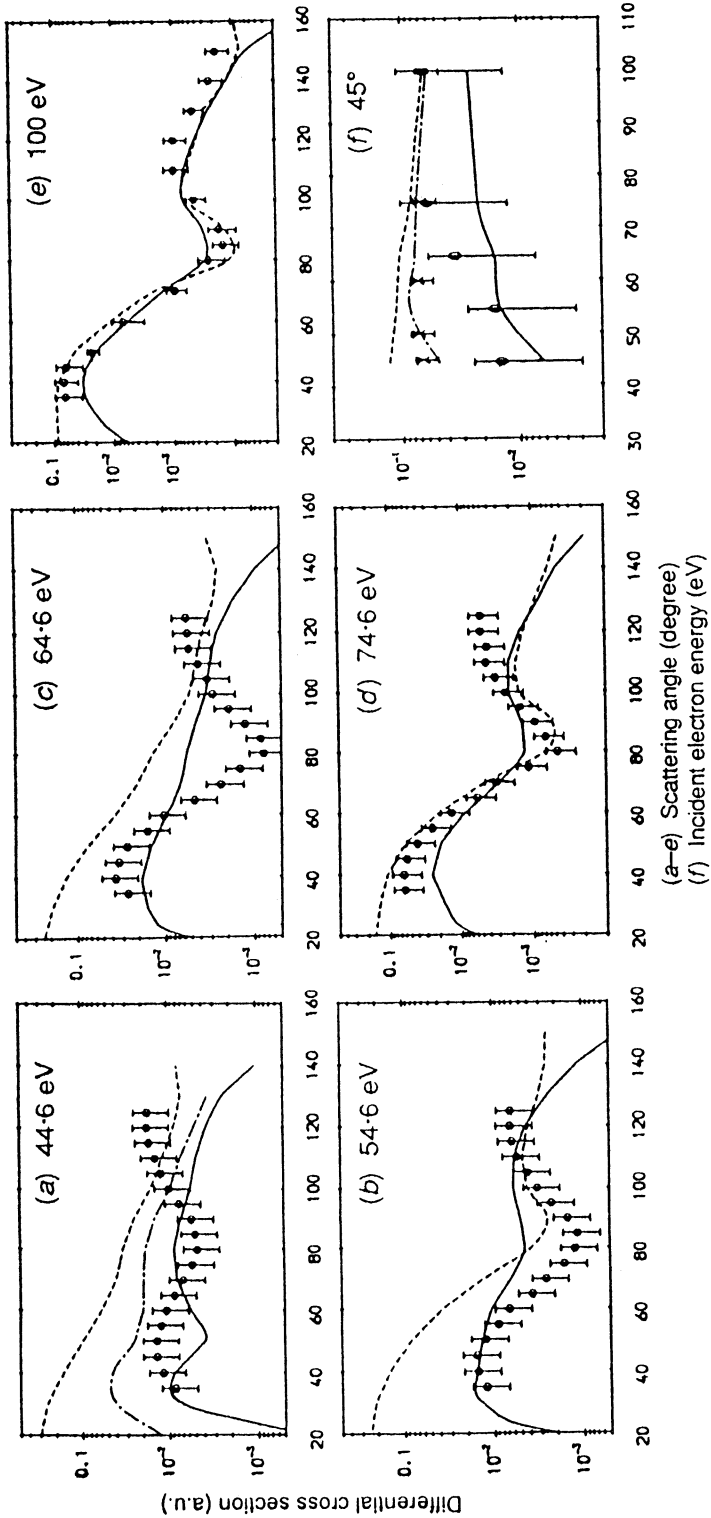
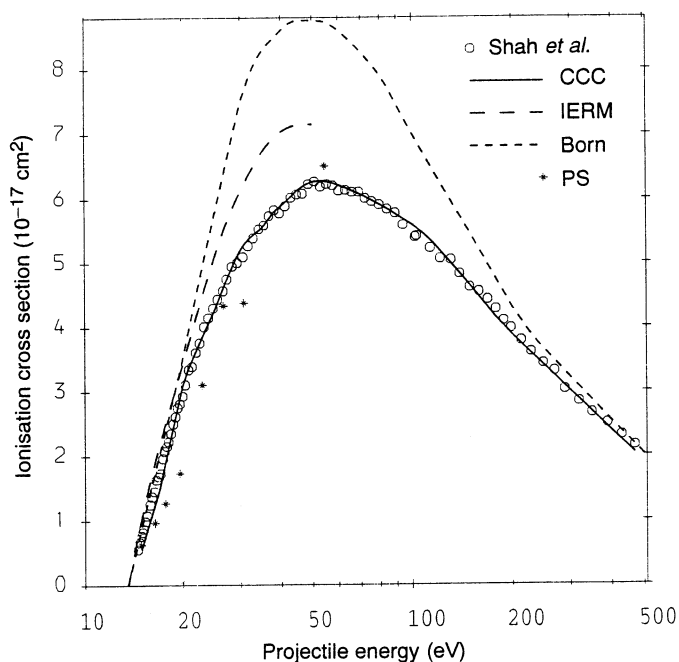
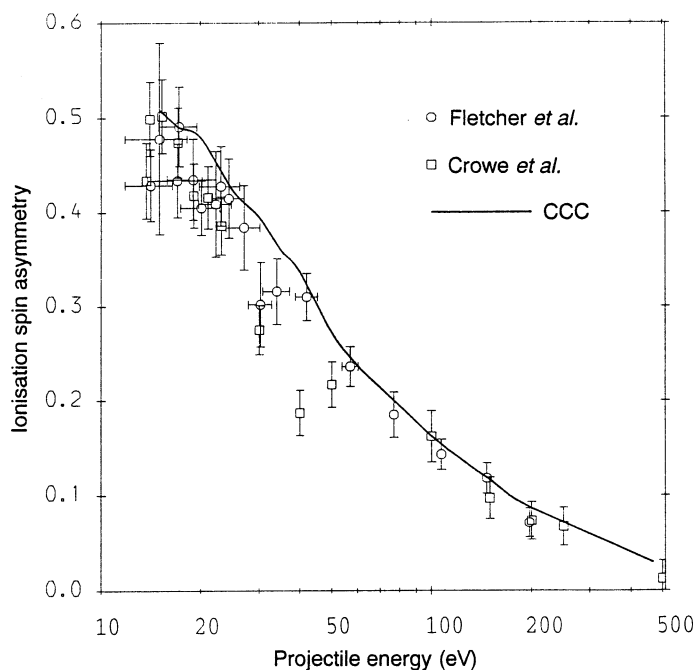


Fig. 2. Coplanar symmetric ionisation of helium. Experimental data are: (a)–(d) Murray and Read (1993); (e) Gélébart and Tweed (1990); (f) absolute 45° differential cross sections measured by Pochat *et al.* (1993), crosses; and Murray and Read (1993), circles. Data in (a)–(e) are normalised to (f). Calculated curves are: BBK, solid; DWBA, short dashes; and equations (19) and (20) [ $\beta = 2$  for (a),  $\beta = 6$  for (f)], chain curve.



**Fig. 3.** Total ionisation cross section for hydrogen. Experimental data: Shah *et al.* (1987). Full curve: CCC (Bray and Stelbovics 1992); plus signs: coupled-channels optical (Bray *et al.* 1991); crosses: pseudostate calculation (Callaway and Oza 1979); long-dashed curve: intermediate-energy *R*-matrix calculation (Scholz *et al.* 1990); and short-dashed curve: DWBA.



**Fig. 4.** Total ionisation asymmetry for hydrogen. Open circles: Fletcher *et al.* (1985); squares: Crowe *et al.* (1990). Full curve: CCC (Bray and Stelbovics 1992); crosses: coupled-channels-optical (Bray *et al.* 1991).

but it is in the BBK approximation, which has the additional advantage in terms of criterion 2 of Section 2 that the ansatz for the unknown function  $\langle \mathbf{r}_1, \mathbf{r}_2 | \Psi^{(-)}(\mathbf{p}_1, \mathbf{p}_2) \rangle$  at least has the correct asymptotic form. BBK maintains the product form for all  $r_1, r_2$ . This is unrealistic in the interior of the atom where the two-electron interaction is strongly screened.

Konovalov and McCarthy (1994) compared DWBA [calculated by setting  $C = 1$  in (19)] and BBK with coplanar symmetric experiments at a range of energies. The results are shown in Fig. 2. At lower energies the explicit treatment of the final-state correlation improves the agreement with experiment for BBK at small angles. At higher energies BBK and DWBA approach each other, with DWBA being slightly superior.

It is likely that the small-distance form of DWBA and the large-distance form of BBK are better choices for  $\langle \mathbf{r}_1, \mathbf{r}_2 | \Phi^{(-)}(\mathbf{p}_1, \mathbf{p}_2) \rangle$ . Konovalov and McCarthy used the form for the final state correlation factor

$$C_\beta(\eta, \mathbf{k}, \mathbf{r}) = e^{-(r_1^2 + r_2^2)/\beta^2} + (1 - e^{-(r_1^2 + r_2^2)/\beta^2})C(\eta, \mathbf{k}, \mathbf{r}), \quad (20)$$

which is BBK for small  $\beta$  and DWBA for large  $\beta$ . Fig. 2a shows that  $\beta = 2$  gives cross sections between the two extremes, but that (20) gives no real hope of finding a simple approximation that enlarges the range of validity of DWBA.

## 7. The Convergent Close-coupling Method

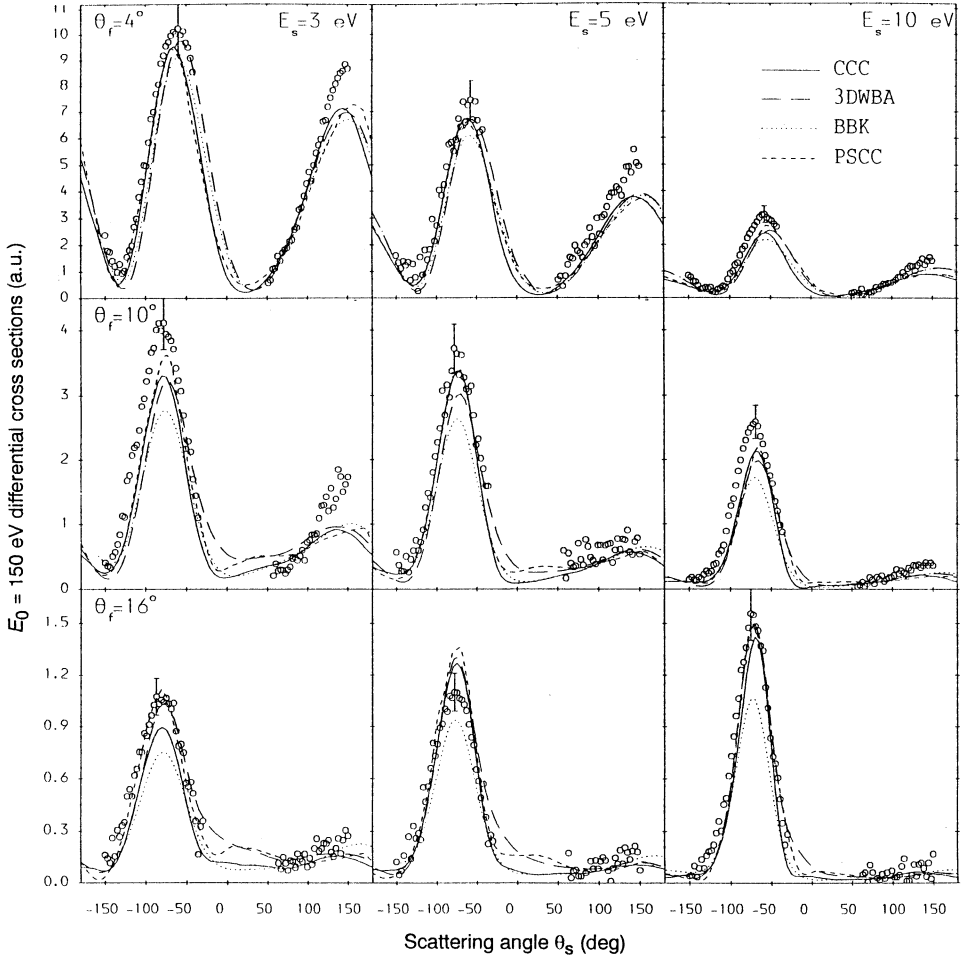
The CCC method (Bray and Stelbovics 1992) assumes that the potential  $V$  is of short range. The  $T$ -matrix element (11) is given by the solution of a Lippmann-Schwinger equation obtained by substituting (9) in (11), using closure over distorted-wave channel states and the definition (8) of the  $T$ -matrix element for discrete states. The sum over target states  $\beta$  implicitly includes ionised states, where it is a discrete notation for the continuum:

$$\begin{aligned} \langle \mathbf{p}_1 \mathbf{p}_2 | T | \alpha \mathbf{p}_0 \rangle &= \langle \chi^{(-)}(\mathbf{p}_1) \chi^{(-)}(\mathbf{p}_2) | V - U_1 | \alpha \chi^{(+)}(\mathbf{p}_0) \rangle \\ &+ \Sigma_\beta \int d^3 p \langle \chi^{(-)}(\mathbf{p}_1) \chi^{(-)}(\mathbf{p}_2) | V - U_1 | \beta \chi^{(-)}(\mathbf{p}) \rangle \\ &\times \frac{1}{E^{(+)} - \epsilon_\beta - \frac{1}{2}p^2} \langle \mathbf{p} \beta | T | \alpha \mathbf{p}_0 \rangle. \end{aligned} \quad (21)$$

The method approximates the Hamiltonian operator of the target by a finite, discrete matrix representation using an orthonormal basis of Laguerre functions. In the case of hydrogen it is a single-particle basis. The range parameter of the Laguerre functions is adjusted for each orbital angular momentum so that one eigenstate has the experimental energy  $E_s$ . Convergence is achieved in the number of partial waves included in the description of the target and in the dimension of the Laguerre basis for each partial wave.

The method was first tested as an overall description of the ionisation of hydrogen by comparing its results for the total ionisation cross section and asymmetry with experiment. These are shown in Figs 3 and 4 respectively. The results of other theoretical methods, including DWBA, are shown for comparison. CCC describes the data essentially perfectly at all energies.



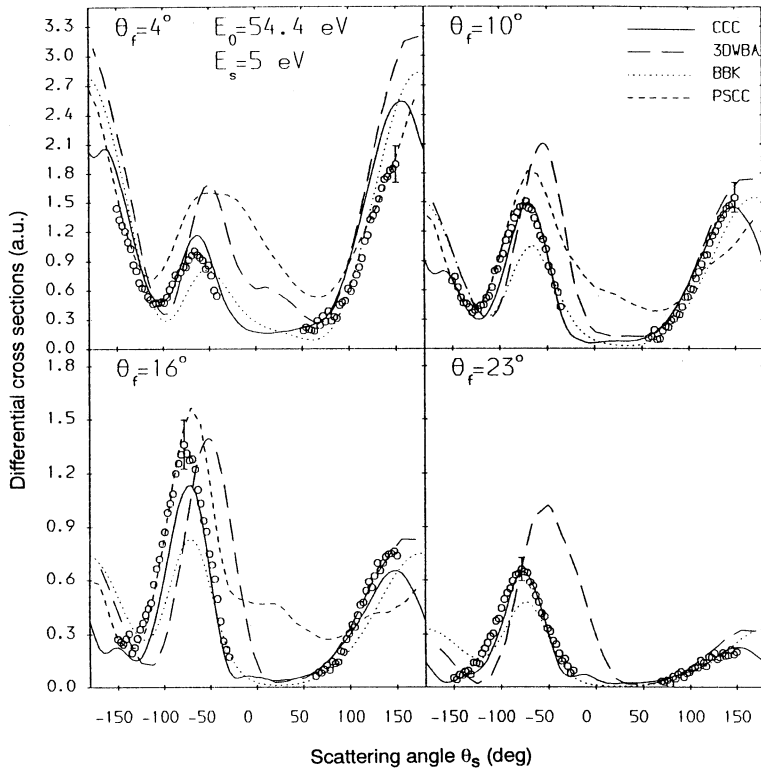


**Fig. 5.** Differential cross section for the coplanar asymmetric ionisation of hydrogen at  $E_0 = 150$  eV. Experiment: Ehrhardt *et al.* (1986). CCC: Bray *et al.* (1994); 3DWBA: Jones *et al.* (1993); BBK: Brauner *et al.* (1989); and PSCC: Curran *et al.* (1991).

For the differential cross section, coplanar asymmetric kinematics is most favourable for the assumption of a short-range potential, since the screening of  $v_1$  by  $v_3$  is more effective if  $E_s \ll E_f$ . Exchange terms in this case are negligible and we can equate  $\mathbf{p}_1$  with  $\mathbf{p}_f$ . Figs 5 and 6 compare various calculations with experimental data at 150 and 54.4 eV (Bray *et al.* 1994). CCC describes the data quite well at the higher energy and much better than BBK for both energies.

## 8. Conclusions

Formal considerations of the ionisation problem have not yet led to a universally-valid computational method. The DWBA is valid in many kinematic cases at energies above about 100 eV and sets a high standard for more-detailed calculations. Correct description of the final-state boundary condition does not guarantee improvement over the DWBA in general. Considerable improvement



**Fig. 6.** Differential cross section for the coplanar asymmetric ionisation of hydrogen at  $E_0 = 54.4$  eV. Experiment: relative measurements of Brauner *et al.* (1991). Calculation of the curves is as for Fig. 5.

for coplanar asymmetric kinematics is achieved with a detailed calculation of the three-body problem assuming that the projectile encounters a short-range potential.

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