

Calculation of Electron Scattering on Atoms and Ions*

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Abstract

We present an overview of the application of the convergent close-coupling (CCC) method to electron scattering on light atoms and ions. Particular emphasis is given to those areas where other theories have difficulty, e.g. total ionisation cross sections and the associated spin asymmetries. We begin with the simplest application to the Temkin–Poet model problem of electron–hydrogen scattering, which we use to validate the CCC approach. Subsequently, results are given for electron impact ionisation of various initial states of the targets H(1s, 2s), He($1^1S, 2^{3,1}S$), He⁺(1s), Li(2s), O⁵⁺(2s) and Na(3s).

1. Introduction

Our motivation in developing electron–atom ion scattering theory is to provide accurate cross section data which are required in practical applications. To this end we concentrate our efforts towards general approaches that are applicable to a broad range of projectile energies and variety of targets.

A fundamental problem in all electron scattering systems is that of three bodies interacting via the Coulomb potential. As our targets are either atoms or ions, and there are no bound two-electron states, we make the approximation that the centre of mass is at the nucleus, and expand the total wave function in an appropriately symmetrised complete set of target states (multichannel expansion) with the origin being at the nucleus. Note that this is not appropriate for positron scattering due to the possibility of positronium formation. An additional approximation is that non-relativistic quantum mechanics is assumed to be sufficiently accurate for the targets of interest to us, and so we use the *LS* coupling scheme.

These approximations are the starting point for our theoretical development. Upon a multichannel expansion of the total wave function the resulting electron–target scattering equations take the form of coupled integro-differential equations in configuration space (Percival and Seaton 1957), or coupled integral equations in momentum space (McCarthy and Stelbovics 1983). Perturbative techniques rely on the expansion of these equations in a rapidly convergent series, which

* Refereed paper based on a contribution to the Advanced Workshop on Atomic and Molecular Physics, held at the Australian National University, Canberra, in February 1995.

is only the case at high projectile energies, and so are not appropriate to our needs. Instead, we look to solve the coupled equations directly, without further approximation.

Historically, due to computational limitations, the multichannel expansion was truncated at the first few target states. Techniques were developed for solving the coupled equations, known as the close-coupling (CC) equations, non-iteratively. Such calculations have dominated the application to low projectile energies. As a rough rule the CC methods give relatively accurate results at those projectile energies which are insufficient to excite the omitted target states of the multichannel expansion. However, these methods are often unable to describe accurately any phenomena (e.g. elastic scattering), for targets such as H or He, that are affected by the dipole-polarisability contribution from the target continuum. As such, these techniques are also inappropriate to our needs.

We do not wish to truncate the complete set of target states in the multichannel expansion even though such an expansion contains an infinite set of discrete states and an integral over the continuum. In the convergent close-coupling (CCC) method (Bray and Stelbovics 1992*a*) we replace the infinite multichannel expansion over true target states to a finite sum over square-integrable states obtained by diagonalising the target Hamiltonian in an orthogonal Laguerre basis. This procedure results, as the basis size is increased, in negative energy states that converge pointwise to the true corresponding target eigenstates, and positive energy states that provide a quadrature rule for the integration over the true target continuum (Bray and Stelbovics 1995*a*). The usage of an orthogonal basis ensures that target-space ‘completeness’ is approached with increasing basis size. The problem has then been recast to performing calculations with sufficiently large basis sizes for convergence in the scattering process of interest. Once convergence, to a required accuracy, has been achieved we believe the results are true solutions of the coupled equations generated by the use of the complete set of true target discrete and continuous eigenstates.

2. Overview of the CCC Theory

The details of the CCC theory for the e-H scattering were given by Bray and Stelbovics (1992*a*). The CCC theory was then extended to hydrogenic targets (Bray 1994*b*), and then to the helium atom (Fursa and Bray 1995). A detailed review of the application of the CCC theory to hydrogenic targets with relation to other theories has been given by Bray and Stelbovics (1995*b*). For detailed technical information the reader is referred to these papers. Here we shall give the important steps in setting up the CCC formalism for the calculation of electrons scattering on light atoms or ions.

The first step is to define the target Hamiltonian H_T . We shall use the convention that the projectile electron-space is denoted by the index 0, and the target electrons by numbers. In the case of hydrogenic targets we may write

$$H_T = K_1 + V_1, \quad (1)$$

where K_1 is the one-electron kinetic energy operator and V_1 is the electron-core potential. In the case of true one-electron targets we have $V_1 = -Z/r_1$, otherwise we approximate it by the frozen-core Hartree-Fock potential (Bray 1994*b*). In

the case of helium-like targets we have

$$H_T = K_1 + V_1 + K_2 + V_2 + V_{12}, \quad (2)$$

where V_{12} is the electron-electron potential. In either case we obtain our orthonormal target-space expansion set of states Φ_n^N by diagonalising H_T in an appropriately chosen orthogonal Laguerre basis (of size N) via

$$\langle \Phi_{n'}^N | H_T | \Phi_n^N \rangle = \epsilon_n^N \delta_{n'n}. \quad (3)$$

Having defined the target Hamiltonian we write the total Hamiltonian H as

$$H = H_T + K_0 + V_p, \quad (4)$$

where

$$V_p = V_0 + \sum_{i=1}^{n_e} V_{0i}, \quad (5)$$

and where $n_e = 1$ for hydrogen-like targets, and $n_e = 2$ for helium-like targets. The total wave function $|\Psi^{(+)}\rangle$, which is antisymmetric and has outgoing spherical-wave boundary conditions, satisfies the Schrödinger equation

$$(E - H)|\Psi^{(+)}\rangle = 0, \quad (6)$$

where E is the total energy of the system.

To solve (6) we expand $|\Psi^{(+)}\rangle$ using an explicitly antisymmetric multichannel expansion

$$|\Psi^{(+)}\rangle \approx |\Psi^{N(+)}\rangle \quad (7)$$

$$= (1 - \sum_{i=1}^{n_e} P_{0i}) |\psi^{N(+)}\rangle \quad (8)$$

$$= (1 - \sum_{i=1}^{n_e} P_{0i}) \sum_{n=1}^N |\Phi_n^N f_n^{N(+)}\rangle, \quad (9)$$

where the P_{0i} are the exchange (coordinate and space) operators, and $|f_n^{N(+)}\rangle = \langle \Phi_n^N | \psi^{N(+)} \rangle$. For $n_e > 1$ total antisymmetry (coordinates 0, 1, 2) is ensured as the Φ_n^N must already be antisymmetric. We rely on the completeness of the Laguerre basis so that

$$\lim_{N \rightarrow \infty} |\Psi^{N(+)}\rangle = |\Psi^{(+)}\rangle. \quad (10)$$

Utilisation of the expansion (8) allows us to work with the unsymmetrised

function $|\psi^{N(+)}\rangle$, however, at a cost of its non-uniqueness. It is clear that any function $|\phi^{N(+)}\rangle$ satisfying

$$(1 - \sum_{i=1}^{n_e} P_{0i})|\phi^{N(+)}\rangle = 0, \quad (11)$$

may be added to $|\psi^{N(+)}\rangle$ without affecting the uniqueness of $|\Psi^{N(+)}\rangle$. The multichannel expansion (9) ensures that the non-uniqueness problem occurs only in the space spanned by the Laguerre basis functions, which describe Φ_n^N . This problem may be addressed numerically by imposing the condition

$$\langle \varphi_\alpha \Phi_n^N | P_{0i} | \varphi^{N(+)} \rangle = -\langle \varphi_\alpha \Phi_n^N | \varphi^{n(+)} \rangle \quad (12)$$

for any one-electron basis function φ_α used to span the Φ_n^N . In other words, we impose the condition that $\varphi^{N(+)}$ be antisymmetric in the space spanned by φ_α . This condition ensures uniqueness since for arbitrary constant β

$$\begin{aligned} \langle \varphi_\alpha \Phi_n^N | (1 - \sum_{i=1}^{n_e} P_{0i}) | \psi^{N(+)} \rangle &= \langle \varphi_\alpha \Phi_n^N | (1 - \sum_{i=1}^{n_e} P_{0i}) (|\psi^{N(+)}\rangle + \beta |\phi^{N(+)}\rangle) \\ &= (1 + n_e) \langle \varphi_\alpha \Phi_n^N | \psi^{N(+)} \rangle \\ &= (1 + n_e) \langle \varphi_\alpha \Phi_n^N | (|\psi^{N(+)}\rangle + \beta |\phi^{N(+)}\rangle) \\ &\Rightarrow |\phi^{N(+)}\rangle = 0, \end{aligned} \quad (13)$$

where we applied (12) to both $|\psi^{N(+)}\rangle$ and $|\psi^{N(+)}\rangle + \beta |\phi^{N(+)}\rangle$. The problem of non-uniqueness, introduced by writing an explicitly antisymmetric expansion (8), is a fundamental one that requires addressing before any substantial calculation may be made. For more details see Stelbovics (1990), Bray and Stelbovics (1992a) and Fursa and Bray (1995). To obtain the coupled electron scattering equations from (6) and (9) we first split the total Hamiltonian to obtain

$$(E - H_T - K_0 - U_0) |\psi^{N(+)}\rangle = \left(V_p - U_0 + (E - H) \sum_{i=1}^{n_e} P_{0i} \right) |\psi^{N(+)}\rangle, \quad (14)$$

where, for asymptotic charge Z_a , the asymptotic potential is $U_0 = -Z_a/r_0$. In fact we may also employ short-range distorting potentials within the CCC formalism, which serve to reduce computational resources in solving the coupled equations (Bray 1994b). The asymptotic projectile Hamiltonian is used to define the plane/Coulomb waves (including bound states) $|\mathbf{k}^{(\pm)}\rangle$ by

$$(\epsilon_k - K_0 - U_0) |\mathbf{k}^{(\pm)}\rangle = 0. \quad (15)$$

The boundary conditions $|\Phi_n^N \mathbf{k}_n^{(+)}\rangle$ may then be obtained from

$$0 = (E - \epsilon_n^N - K_0 - U_0) |\Phi_n^N \mathbf{k}_n^{(+)}\rangle = (E - \epsilon_n^N - \epsilon_{k_n}) |\Phi_n^N \mathbf{k}_n^{(+)}\rangle. \quad (16)$$

If we write

$$V = V_p - U_0 + (E - H) \sum_{i=1}^{n_e} P_{0i}, \quad (17)$$

then we may use (14) to obtain the coupled Lippmann-Schwinger equations for the T -matrix

$$\langle \mathbf{k}_f^{(-)} \Phi_f^N | T | \Phi_i^N \mathbf{k}_i^{(+)} \rangle = \langle \mathbf{k}_f^{(-)} \Phi_f^N | V | \psi_i^{N(+)} \rangle \quad (18)$$

$$= \langle \mathbf{k}_f^{(-)} \Phi_f^N | V | \Phi_i^N \mathbf{k}_i^{(+)} \rangle + \sum_{n=1}^N \sum_{\epsilon_k}^f \frac{\langle \mathbf{k}_f^{(-)} \Phi_f^N | V | \Phi_n^N \mathbf{k}^{(-)} \rangle \langle \mathbf{k}^{(-)} \Phi_n^N | T | \Phi_i^N \mathbf{k}_i^{(+)} \rangle}{E + i0 - \epsilon_n^N - \epsilon_k}. \quad (19)$$

These are the coupled integral equations which are solved in the CCC method using the partial-wave formalism, without approximation, to a desired numerical accuracy (typically 1%). The basis size N is increased until convergence in the required T -matrix element $\langle \mathbf{k}_f^{(-)} \Phi_f^N | T | \Phi_i^N \mathbf{k}_i^{(+)} \rangle$, in the case of discrete transitions, is obtained. In the case of (e, 2e), we look for convergence in $\langle X_f^{(-)} | \Phi_f^N \rangle \langle \mathbf{k}_f^{(-)} \Phi_f^N | T | \Phi_i^N \mathbf{k}_i^{(+)} \rangle$, where $X_f^{(-)}$ is the continuum eigenfunction of the target Hamiltonian H_T with energy ϵ_f^N .

Total one-electron ionisation cross sections σ_i^S , for particular total spin S , are obtained by essentially summing (over n) the cross sections for those states with $\epsilon_n^N > 0$ (Bray and Stelbovics 1993). In the case of two possible spins $S > S'$ we may define the total ionisation spin asymmetry A_i by

$$A_i = (\sigma_i^{S'} - \sigma_i^S) / \left(\sigma_i^{S'} + \frac{2S+1}{2S'+1} \sigma_i^S \right). \quad (20)$$

It is very important to test the CCC formalism to establish that:

- (i) convergence with increasing N does indeed occur and that
- (ii) the convergence is to the correct result.

To convince ourselves that this is the case we first apply the CCC formalism to a model problem.

3. Temkin-Poet Model

In order to be confident of the validity of our approach we begin with the simplest target, namely atomic hydrogen. This is an ideal target for the testing of electron scattering theories because the target structure is relatively simple, and requires no approximation. The Temkin-Poet model (Temkin 1962; Poet 1981) of this system is the case where all orbital angular momenta are zero in

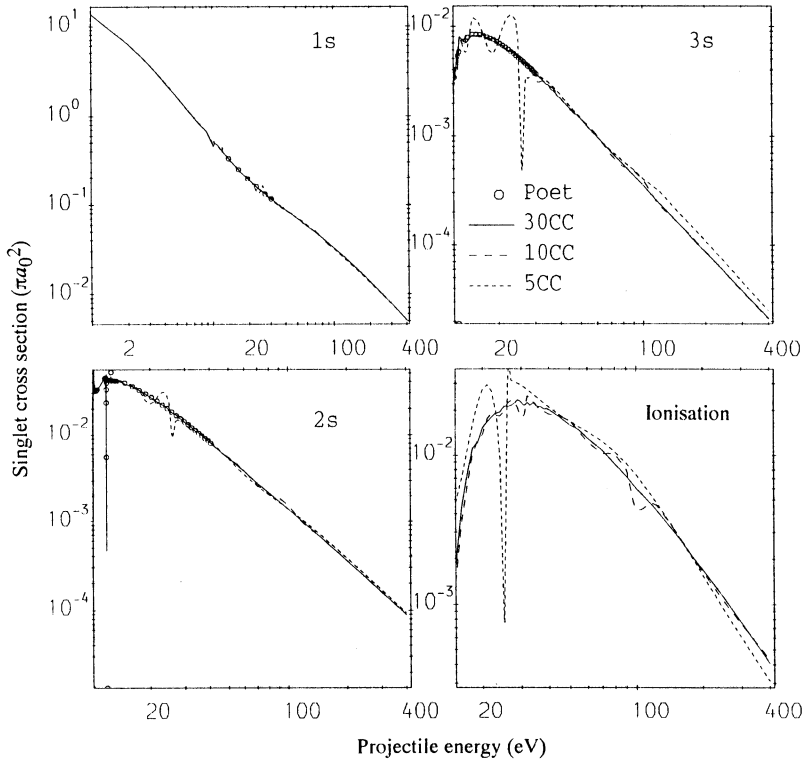


Fig. 1. Singlet cross sections of the simplified (Temkin-Poet) model of electron-hydrogen scattering that treats only states with zero orbital angular momentum. The exact results, denoted by \circ , are due to Poet (1978, 1980). The curves denote close-coupling calculations with 30 (solid curve), 10 (long-dash curve), and 5 (short-dash curve) L^2 states generated using the Laguerre basis (Bray and Stelbovics 1992*b*).

the partial-wave expansion of the full problem. Using techniques particularly suited to this model Temkin and Poet have given a set of accurate benchmark results at a broad range of energies against which we may test the CCC theory. Issues, such as correct symmetrisation and inclusion of the continuum, need to be addressed in order to obtain accurate results for this model problem.

The CCC method was first tested against this model by Bray and Stelbovics (1992*b*). A very important conclusion was able to be drawn from this work. It is that, irrespective of energy, as the basis size increases the CCC results converge to the true result for this model problem, see Fig. 1. We rely on this observation in application of the CCC theory to full electron scattering problems. A consequence of this conclusion is that pseudo-resonances, such as those apparent in pseudo-state methods (Callaway 1985; van Wyngaarden and Walters 1986), are simply an indication of an insufficiently large basis size. To demonstrate this explicitly Bray and Stelbovics (1995*a*) presented a study of the singlet $1s$, $2s$, $3s$ and ionisation cross sections at a small energy range, reproduced here in Fig. 2. We see that for the two smaller basis sizes there is a pseudo-resonance associated with a corresponding pseudo-threshold. The magnitude of the pseudo-resonances

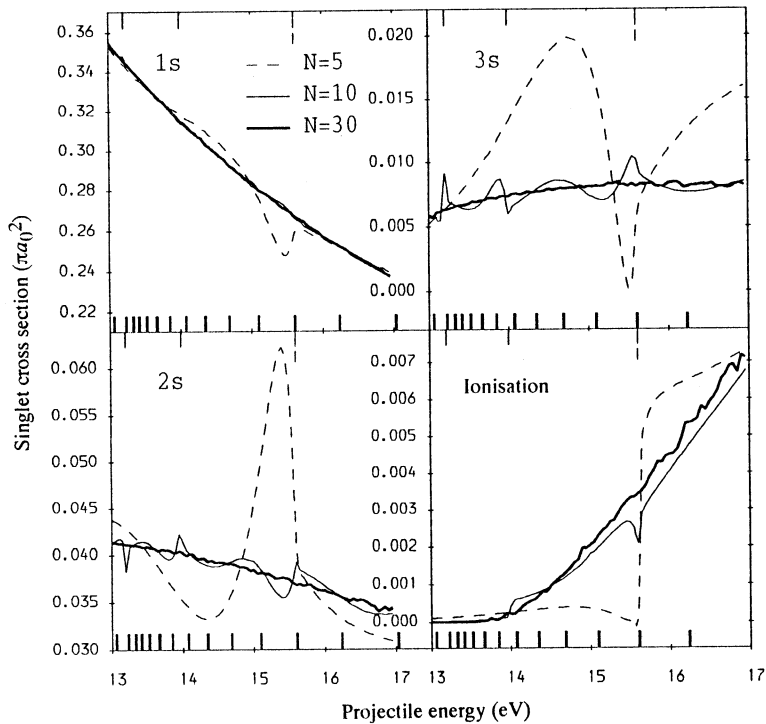


Fig. 2. The 1s, 2s, 3s, and ionisation singlet cross sections in the Temkin-Poet model are shown in a small energy range for three basis sizes. The large 'pips' on the top and bottom horizontal axes indicate energy thresholds corresponding to the basis size indicated. For a given incident energy E , states corresponding to thresholds less than E are open and those greater than E are closed. All three basis sizes lead to a pseudo-threshold at 15.6 eV (Bray and Stelbovics 1995a).

diminishes and disappears with increasing basis size, even in the vicinity of the fixed pseudo-threshold at 15.6 eV.

This model continues to be used as a test case for general electron scattering theories. Watanabe *et al.* (1993) have used it to test the hyperspherical close-coupling (HPCC) method for the discrete excitations. The same was done by Konovalov and McCarthy (1994) to test their J -matrix techniques. The HPCC method was then applied by Kato and Watanabe (1995) to the calculation of the total ionisation cross section for this model, which was found to be in complete agreement with that obtained in the CCC method (Bray and Stelbovics 1992b). The most recent application (Meyer *et al.* 1995) tested the eigenchannel R -matrix approach by application to this model for both e-H and e-He⁺ scattering systems, and obtained good agreement with the CCC method for excitation and ionisation cross sections. Together, these results give us great confidence that the CCC method is able to obtain correct solutions of the Schrödinger equation (6) for elastic, excitation and ionisation processes.

4. CCC Calculations of Electron Impact Ionisation

We now proceed to give a systematic study of electron impact ionisation for a number of targets. We concentrate here on ionisation so as to demonstrate

succinctly that the CCC method is able to calculate simultaneously most scattering processes of interest. Due to unitarity of the close-coupling formalism it is highly unlikely that we would calculate accurate ionisation, but not elastic or excitation processes. A further advantage of looking at such cross sections, or indeed any integrated cross sections, is that we may demonstrate the validity of the method from the low threshold energy to that of order 1 keV.

In all cases below we are only able to provide cross sections for ejection of the valence electron, often referred to as the direct ionisation process. This cross section, we believe, is calculated very accurately in the CCC method since the frozen-core Hartree-Fock approximation is very good for the targets presented. In the following we suggest that the direct ionisation cross sections have been obtained to an accuracy of better than 10%. This has been achieved by expanding the 'one-electron' targets' space with $0 \leq l \leq 4$ and bases sizes $N_l \leq 15 - l$. Typical CCC calculations solve the close-coupling equations with around 50 states, roughly half of which lie in the discrete spectrum and half in the continuum. The case of e-He scattering shall be discussed separately, where calculations with up to 75 states have been performed.

(4a) *Electron-Hydrogen Scattering*

Having demonstrated the validity of the CCC method by application to a model problem, we now turn to the full electron-hydrogen scattering problem. In this case we are only able to test the reliability of the theory by comparison with experiment. Here we immediately run into a problem since as yet no theory is able to describe the complete set of backward angle measurements available for the 2p excitation at 54.4 eV (Bray and Stelbovics 1992a). This is a very long standing problem that we do not wish to overemphasise. Given the many successes of the CCC method for similar measurements in the case of sodium (Bray 1994b) and helium (Fursa and Bray 1995), we argue that in this case it is the theory that is more accurate than the very difficult experiment.

The total ionisation cross section of the e-H(1s) scattering system is known very accurately (error of order 3%). Total ionisation spin asymmetries have also been measured, as have triple and single differential cross sections. The CCC theory is able to obtain very good agreement with most of these measurements (Bray and Stelbovics 1993; Bray *et al.* 1994; Konovalov *et al.* 1994). In Fig. 3 we reproduce the total ionisation results of Bray and Stelbovics (1993). The quality of agreement between the CCC theory and experiment here indicates to us that we have correctly implemented the CCC method to the full e-H problem, and that for this system we are able to calculate correct spin-dependent elastic, excitation and ionisation processes, irrespective of the projectile energy.

The total ionisation cross section of the metastable H(2s) by electron impact is also known relatively accurately (Defrance *et al.* 1981b). In Fig. 4 we present the e-H(2s) total ionisation cross section, and for completeness, the associated spin asymmetry. We find the agreement between the CCC theory and experiment to be very good. This is what we would expect because the e-H(2s) and e-H(1s) results are not independent. In fact in the CCC method we calculate e-H(1s, 2s) simultaneously. We shall see that in the case of e-He(1^1S , $2^3,1S$) ionisation, we only obtain agreement with measurements of e-He(1^1S) ionisation, but not

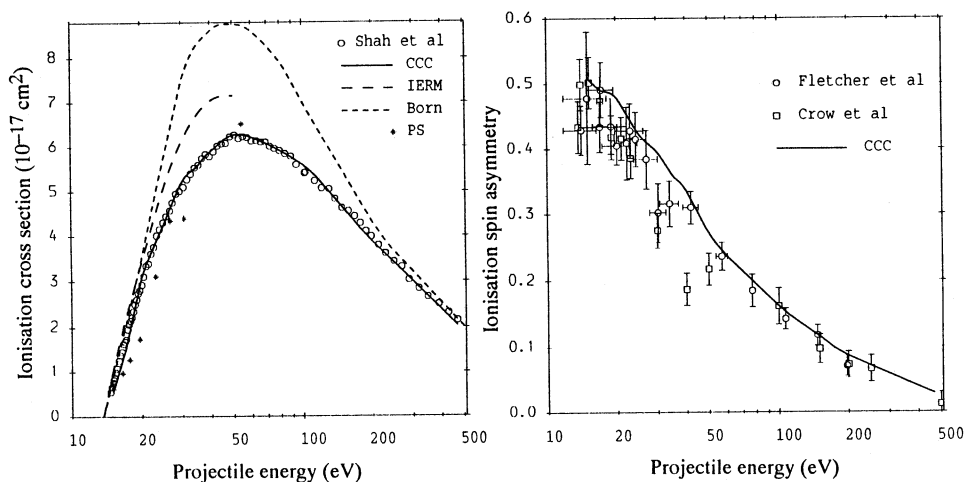


Fig. 3. Total ionisation cross section and spin asymmetry for electron impact of atomic hydrogen. The total ionisation measurements of Shah *et al.* (1987) are denoted by \circ . The spin asymmetry measurements denoted by \circ and \square are due to Fletcher *et al.* (1985) and Crowe *et al.* (1990), respectively. The IERM results are due to Scholz *et al.* (1990), and the pseudostate (PS) results to Callaway and Oza (1979). The convergent close-coupling results (Bray and Stelbovics 1993) are denoted by CCC.

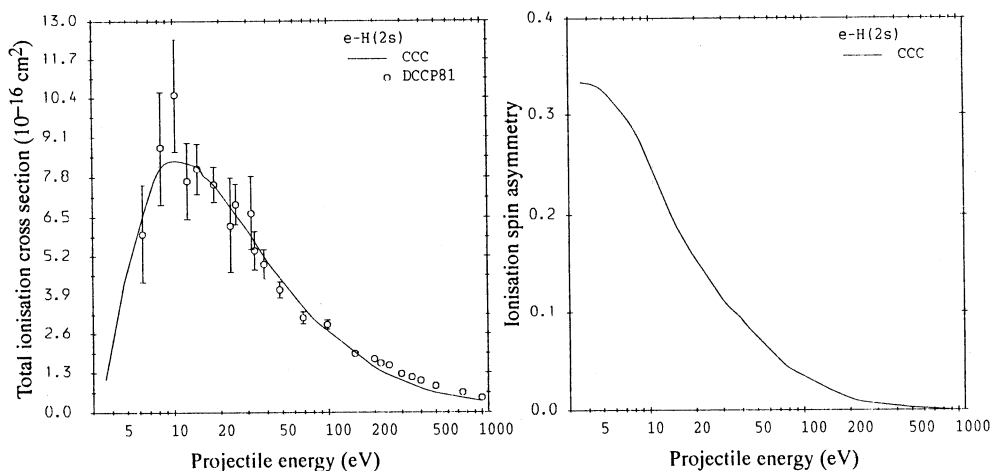


Fig. 4. Total ionisation cross section and spin asymmetry for electron impact of atomic hydrogen in the $2s$ initial state. The total ionisation measurements of Defrance *et al.* (1981*b*) are denoted by \circ . The convergent close-coupling results are denoted by CCC.

$e\text{-He}(2^3S)$. This suggests to us that the latter measurements are less accurate than the CCC theory.

There are no available measurements of $e\text{-H}(2s)$ total ionisation spin asymmetries. It is interesting to note the similarity with the $e\text{-H}(1s)$ results. They are qualitatively the same, though there is a small drop in the magnitude.

(4b) Electron-Helium Ion Scattering

Having satisfied ourselves that the CCC method is able to solve the fundamental electron-atom scattering problem, we turn our attention to the fundamental electron-ion scattering problem. The change of target from H to He^+ requires the introduction of the long-range asymptotic potential $U_0 = -1/r_0$, see equation (14). Bray *et al.* (1993b) applied the CCC method to the calculation of total ionisation and $2s$ excitation. The former were in excellent agreement with experiment, see Fig. 5. The latter were in very good agreement with experiment for the energy range of a few eV above threshold. Near the threshold region the CCC theory is considerably above the available $2s$ excitation measurements, but is in agreement with other theory. As in the case of atomic hydrogen, no approximations are necessary for the target structure. Having readily established convergence we suppose that the CCC theory is equally reliable across the entire energy range. We do not expect that the formal approximations outlined in the introduction are responsible for any discrepancies between experiment and the CCC calculations of electron scattering on H or He^+ .

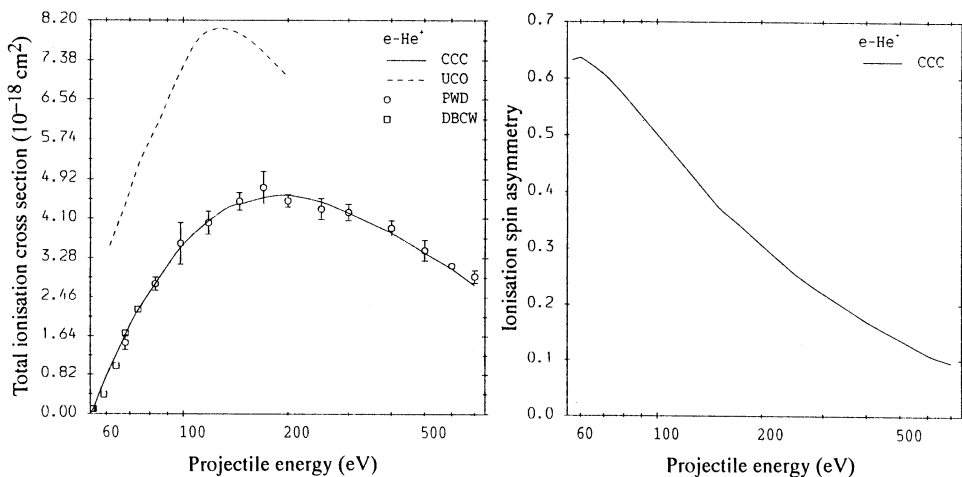


Fig. 5. Total ionisation cross section and spin asymmetry of the ground state of He^+ by electron impact. The calculations of Unnikrishnan *et al.* (1991) are denoted by UCO. The measurements of Peart *et al.* (1969) and those of Defrance *et al.* (1981a) are denoted by PWD and DBCW, respectively. The convergent close-coupling results (Bray *et al.* 1993b) are denoted by CCC.

(4c) Electron-Lithium Scattering

Having applied the CCC method to two cases of true one-electron targets, we now consider hydrogenic targets, those which may be readily treated by the frozen-core Hartree-Fock approximation. With the aid of this approximation we reduce the full scattering to a model three-body problem. Demonstrating convergence in the CCC calculations leads to the solution of this model problem—how close the solution is to the true result is problematical. What we can say is

that the CCC results solve the Schrödinger equation (6) without approximation. The question is how accurate is the frozen-core Hartree-Fock description of the interaction of the core electrons and an external electron. To test this approximation we compare the energy levels obtained for the hydrogenic target structure. If these are accurate enough then we are able to calculate processes such as elastic, excitation, and one-electron ionisation by electron impact of the target. We are not able to provide results for ejection of two, or more, electrons.

Until recently (Bray 1995) we have only the coupled-channels optical (CCO) method to electron-lithium scattering (Bray *et al.* 1993a). This method can be viewed as an approximation to the CCC method, which does not allow coupling between distinct positive-energy states, but does allow full coupling in the discrete spectrum, and between discrete and continuum states. This method was able to reproduce elastic and excitation phenomena quite accurately, and we do not expect the CCC method to do significantly better for these transitions. However, due to the approximate nature of the treatment of the continuum in the CCO formalism, the CCC method is much superior for calculating ionisation processes.

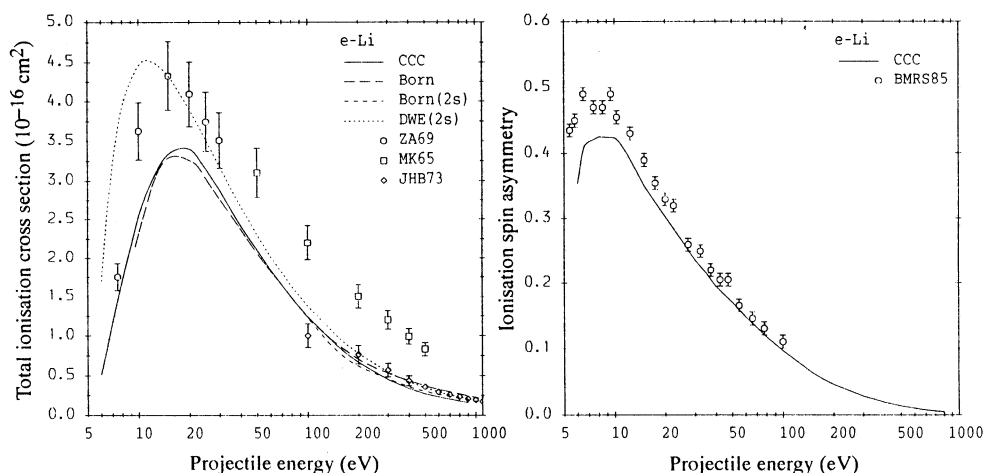


Fig. 6. Total ionisation cross section and spin asymmetry of the ground state of lithium by electron impact. The convergent close-coupling calculations (Bray 1995) for ejection of the 2s electron are denoted by CCC. The Born calculations of McGuire (1971) have an estimate of the contribution due to ejection of a 1s electron. The distorted-wave with exchange calculations of Younger (1981) are denoted by DWE(2s). The measurements of Zapesochnyi and Aleksakhin (1969), McFarlane and Kinney (1965), Jalin *et al.* (1973) and Baum *et al.* (1985) are denoted by ZA69, MK65, JHB73 and BMRS85, respectively.

In Fig. 6 we present the CCC calculations (Bray 1995) of the total one-electron ionisation cross section and the associated spin asymmetries. These are compared with the available experimental data, and Born approximations. Agreement with the most recent measurements of the total ionisation cross section by Jalin *et al.* (1973) is very good. They argued that the earlier measurements suffered from experimental difficulties, and so we can be confident that our results are accurate across the entire energy range. It is interesting to see that the Born approximations of McGuire (1971) yield results similar to the CCC theory. The

difference between the two Born calculations is due to the Born estimate of the contribution to the ionisation from the core electrons, which is barely visible. The semi-empirical distorted-wave with exchange DWE(2s) calculations (Younger 1981) yield significantly different results at the smaller energies. These results have been obtained by taking an empirical relation for the cross section for the ejection of the 2s electron, which has a defined behaviour at both threshold and infinity, and determining a set of coefficients by matching to the distorted-wave with exchange calculations (Younger 1980).

Agreement of the CCC results for the ionisation spin asymmetries with the measurements of Baum *et al.* (1985) is quite good, but not perfect. It is difficult to determine what is the cause of the minor discrepancy. We shall see that we obtain even better agreement with the corresponding measurements in the case of the sodium target. This suggests that the discrepancy is not likely to be due the frozen-core approximation. Note that Born approximations are independent of total spin and so yield identically zero for the ionisation spin asymmetry.

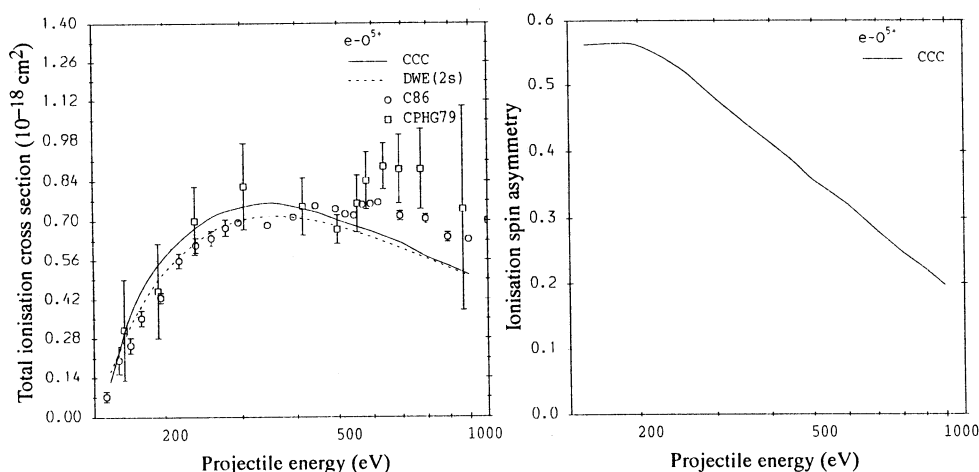


Fig. 7. Total ionisation cross section and spin asymmetry of the ground state of O^{5+} by electron impact. The convergent close-coupling calculations for ejection of the 2s electron are denoted by CCC (Bray 1995). The DWE(2s) calculation is due to Younger (1981). The measurements of Crandall *et al.* (1979, 1986) are denoted by CPHG79 and C86, respectively.

(4d) Electron Impact Ionisation of O^{5+}

In the work on electron-impact ionisation of lithium-like targets (Bray 1995) we found an interesting aspect that we would like to reproduce here. We found that as the ionic charge increases so does the ionisation spin asymmetry at higher energies. In Fig. 7 we present the ionisation results for electron impact ionisation of O^{5+} . The spin asymmetry, $A_i = (1 - r)/(1 + 3r)$, where r is the ratio of triplet to singlet total ionisation cross sections (see equation 20), takes the large value of 0.2 at the projectile energy of 1 keV. This implies $r = 0.5$, or that singlet scattering is twice the magnitude of triplet scattering, at this very high energy. The reason for this is simple. The size of the lithium-like ion diminishes with

increasing ionic charge. The ionisation cross section then becomes dominated by electron collisions with small impact parameter, i.e. low partial waves in the CCC theory. For such collisions exchange plays an important role leading to a larger spin asymmetry. It is interesting to compare these results with those of Fig. 6.

Turning to the total ionisation cross section results, we see that we get good agreement with experiment at energies below core excitation. This indicates the limitation of the 'one-electron' model that the CCC method uses in describing lithium-like targets. Note that the magnitude of this cross section is considerably lower than that in the case of lithium.

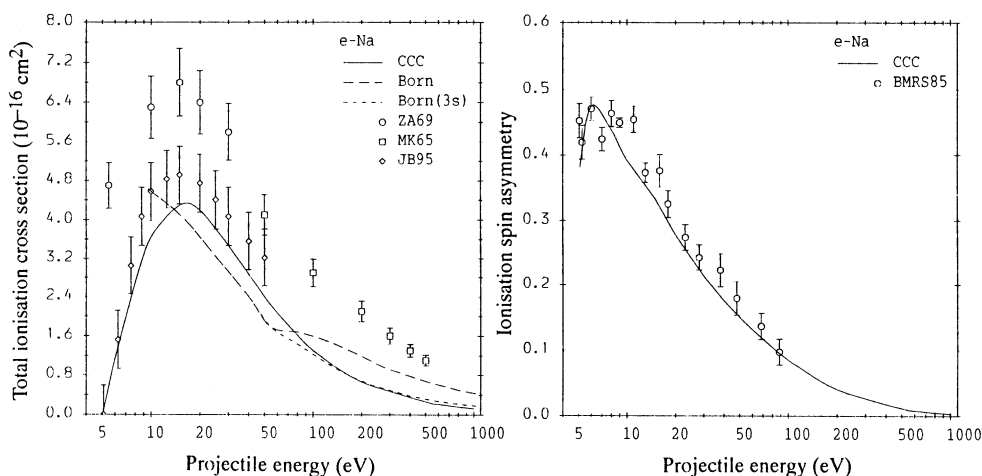


Fig. 8. Total ionisation cross section and spin asymmetry of the ground state of sodium by electron impact. The convergent close-coupling calculations (Bray 1994a) for ejection of the 3s electron are denoted by CCC. The born calculations of McGuire (1971) have an estimate of the contribution due to ejection of a 2p electron. The measurements of Zapesochnyi and Aleksakhin (1969), McFarland and Kinney (1965), Johnston and Burrow (1995) and Baum *et al.* (1985) are denoted by ZA69, MK65, JB95 and BMRS85, respectively.

(4e) Electron Impact Ionisation of Na

One interesting aspect of the calculation of total ionisation cross sections via the close-coupling formalism is that unitarity allows us to obtain convergence in the cross sections without requiring convergence in individual partial contributions for each target state orbital angular momentum l . We demonstrated this in the case of e-Na ionisation for the cases where the incident state is either 3S or 3P (Bray 1994a). However, even though convergence in the total ionisation cross section was obtained, the CCC results were a factor of two less than the available experiment. Since that time Johnston and Burrow (1995) have reported measurements which are in much better agreement with our results. These are given in Fig. 8 together with the earlier measurements and the Born results of McGuire (1971). The latter also estimated the contribution to the ionisation cross section from ejection of a 2p electron. This is significant at larger energies. Note that the CCC and the Born(3s) calculations are very similar at the large energies, as one would expect. Given the approximate treatment of the sodium

target we are not perturbed by the marginal difference between the CCC results and the latest experiment. The new measurements for the e-Na system give us further confidence in the reliability of our e-Li results at all of the energies presented in Fig. 6.

In Fig. 8 we also find excellent agreement with the measurements of the total ionisation spin asymmetries (Baum *et al.* 1985). In fact it is slightly better than in the case of lithium. Given that the frozen-core approximation is best for the lighter targets we find the marginally better agreement here a little surprising.

(4f) Electron Impact Ionisation of He

The CCC method has been recently extended to the calculation of e-He scattering (Fursa and Bray 1995), with great success. The concept of convergence is a little different to the case of hydrogenic targets, where the target space is spanned by one-electron functions. In the case of the helium target, the target space contains two electrons. However, thus far we have found it to be sufficient to consider only one-electron excitation, and thereby restrict one of the electrons to occupy the $\text{He}^+ 1s$ orbital. Though we found very good agreement with the vast variety of experiments available for electrons scattering from the ground (1^1S) state, not so good agreement was found in the case of scattering from the metastable 2^3S state (Bray and Fursa 1995).

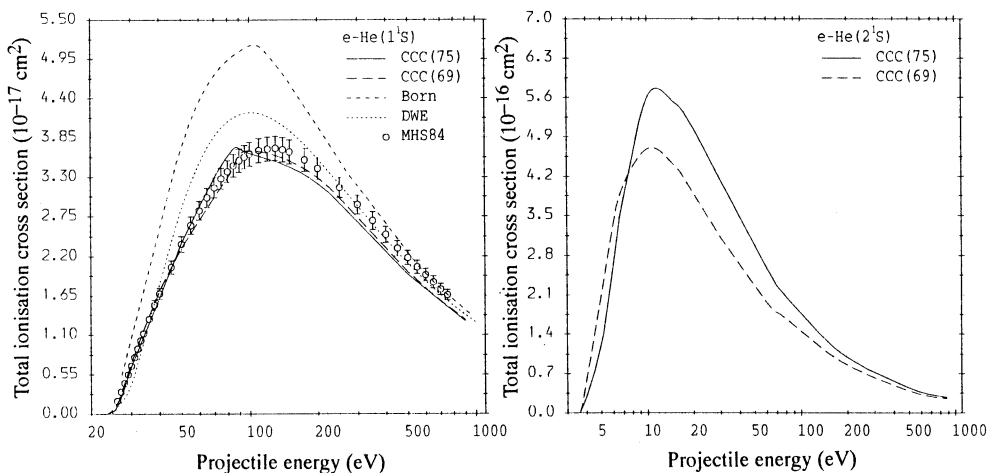


Fig. 9. Total ionisation cross sections of the 1^1S and 2^1S states of helium by electron impact. The convergent close-coupling calculations are denoted by CCC(75) and CCC(69) (Fursa and Bray 1995; Bray and Fursa 1995). The former includes up to $l = 3$ states, whereas the latter includes up to $l = 2$ states in the close-coupling formalism. The Born and DWE calculations are due to McGuire (1971) and Younger (1981), respectively. The measurements of Montague *et al.* (1984) are denoted by MHS84.

In Fig. 9 we present total ionisation cross sections for one-electron ionisation of the 1^1S and 2^1S states of helium by electron impact. As we have not yet presented a convergence study with increasing target-space l , we do so here. Two CCC calculations are presented. One couples a total of 75 states, which includes up to F states, and the other couples 69 states, which has only S , P

and D states, but has more of them than the 75-state calculation (Fursa and Bray 1995). Looking at the 1^1S results first, it is evident that both calculations are in very good agreement with the measurements of Montague *et al.* (1984), and are superior to the Born calculation of McGuire (1971) and the DWE calculation of Younger (1981) at most energies. At the intermediate energies it is clear the 69-state calculation is in marginally better agreement with experiment. This indicates that it is more important to have more S , P and D states than including F states for this process.

This situation is reversed in the case of ionisation from the 2^1S state. Here we have no experiment to compare with, but we see that the effect of F states is quite substantial, and so the 75-state result is likely to be the more accurate. This behaviour is very similar to what we found in the case of ionisation of the $\text{Na}(3p)$ state (Bray 1994a). We expect inclusion of G states is likely to have a marginal increase in the total ionisation cross section. Inclusion of more S , P , D and F states is likely to have an effect of a similar magnitude as in the case of ionisation of the helium ground state.

The results for ionisation of the 2^3S state of helium are given in Fig. 10. In the case of the total ionisation cross section we find that the convergence considerations are identical to the case of ionisation from the 2^1S state. The discrepancy between the 75-state calculation and the experiment of Dixon *et al.* (1976) is not likely to be due to convergence problems. This is particularly evident when we look at the ionisation spin-asymmetry results, which are less sensitive to the inclusion of F states, and give an excellent account of the data of Baum *et al.* (1989). The fact that we calculate $\text{e-He}(1^1S, 2^3, 1^1S)$ simultaneously, and

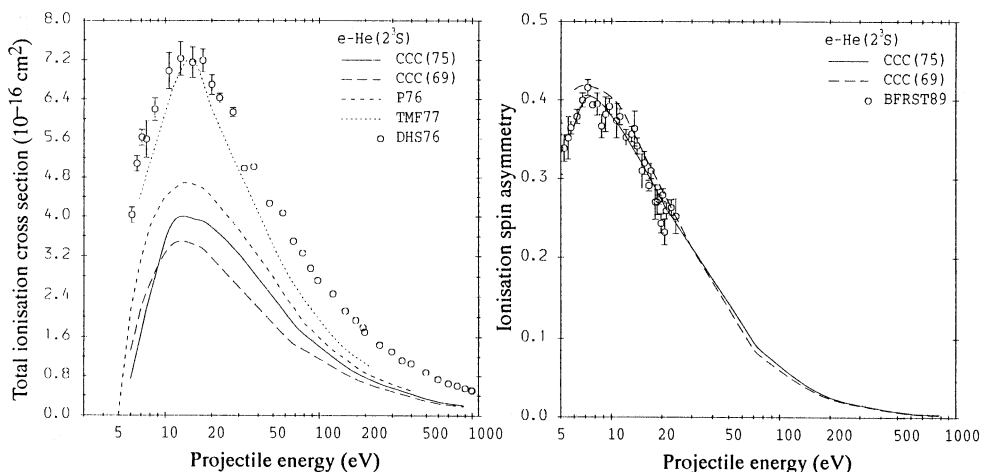


Fig. 10. Total ionisation cross section and spin asymmetry of the 2^3S state of helium by electron impact. The convergent close-coupling calculations are denoted by CCC(75) and CCC(69) (Bray and Fursa 1995). The former includes up to $l = 3$ states, whereas the latter includes up to $l = 2$ states in the close-coupling formalism. The calculations of Ton-That *et al.* (1977) are denoted by TMF77, and those of Peach (Dixon *et al.* 1976) are denoted by P76. The measurements of Dixon *et al.* (1976) and those of Baum *et al.* (1989) are denoted by DHS76 and BFRST89, respectively.

that we obtain the correct e-He(1^1S) total ionisation cross sections and correct e-He(2^3S) spin asymmetries, suggest that the CCC e-He(2^3S) total ionisation cross sections are also reliable. Dixon *et al.* (1976) also presented a number of Born-based approximations for the measured cross section. Whereas these vary in their predictions at the lower energies, as expected, they converge to the CCC results at the higher energies.

5. Conclusions

We have demonstrated the generality of the CCC formalism by applying it to a range of targets at a range of projectile energies. We are confident, that in the cases where substantial discrepancy with experimental data has been demonstrated, that it is the CCC theory which is likely to be the most accurate. This is because the primary, frozen-core approximation is very accurate for the targets considered. Having made this approximation, the coupled equations are solved to an accuracy which may be examined by checking the convergence of the CCC calculations with ever increasing basis sizes.

Application of the method to ionisation of lithium-like ions has been recently completed (Bray 1995). This will be followed by application to sodium-like ions. The next stage in the development of the CCC method is to extend it to incorporate helium-like atoms and ions.

Acknowledgments

The author is grateful to Dmitry Fursa, Ian McCarthy and Andris Stelbovics for a number of useful discussions. Support of the Australian Research Council and the Flinders University of South Australia is acknowledged.

This research was sponsored in part by the Phillips Laboratory, Air Force Material Command, USAF, under cooperative agreement number F29601-93-2-0001. The views and conclusions contained in this document are those of the author and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of Phillips Laboratory or the US Government.

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