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To cite this article: I Bray *et al* 2010 *J. Phys.: Conf. Ser.* **212** 012017

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Spin-resolved electron-impact ionisation of atoms

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Abstract. We shall consider various aspects of electron-impact ionisation of atoms. Firstly, the recent progress in the formulation of the problem will be outlined. Then application of the convergent close-coupling (CCC) method to the calculation of the total ionisation spin asymmetries will be described for a range of neutral through to highly charged targets. We shall also consider the importance of electron spin in the problem of single and double photoionisation of lithium. Lastly, application of the CCC method to 64.6 eV e-He ionisation fully differential cross sections for in- and out-of-plane geometries will be considered.

1. Introduction

There has been much progress during the last decade in the theoretical treatment of electron-impact ionisation of atoms and the closely related problem of double photoionisation. The existence of readily accessible super-computer facilities has allowed the application to the problem of numerically intensive techniques that essentially solve the Schrödinger equation with minimal approximation. These are either based on the exterior complex scaling (ECS) approach [1–4] or the close-coupling method, time-independent [5–9] or time-dependent [10, 11]. Whereas total ionisation cross sections can be obtained from unitary theories utilising just the excitation amplitudes [12], when it comes to differential cross sections an ionisation amplitude is required. How that can be rigorously defined, even when the total wavefunction is available, has been problematic until very recently [13, 14]. Despite this an excellent agreement with experiment for fully differential cross sections has been obtained for quite some time, see for example [2, 8, 9]. So we have a very unusual situation where accurate agreement with experiment for fully differential ionisation cross sections has been obtained before it was clear how to go about calculating the underlying ionisation amplitudes. We begin by considering this question.

2. Surface-integral formulation of scattering theory

Few-body break-up problems involving long-range Coulomb potentials have been of interest for many decades. Yet even the two-body problem has not had an adequate mathematical formulation. Methods involving screening require renormalization due to singularities in the resultant on-shell amplitudes, see Kadyrov *et al* [14] and references therein for a detailed discussion. While the resolution of these problems is rather detailed and complicated, here we give just the underlying ideas.

Starting with a two-body scattering problem, for Hamiltonian $H = H_0 + V$ we write the Schrödinger equation

$$(\epsilon - H)\psi_{\mathbf{k}}^{\pm}(\mathbf{r}) = 0. \quad (1)$$

If V is short-ranged then

$$\psi_{\mathbf{k}}^+(\mathbf{r}) \stackrel{r \rightarrow \infty}{\sim} e^{i\mathbf{k} \cdot \mathbf{r}} + f(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}})e^{ikr}/r, \quad (2)$$

or if V is long-ranged, i.e. Coulomb, then

$$\begin{aligned} \psi_{\mathbf{k}}^+(\mathbf{r}) \stackrel{r \rightarrow \infty}{\sim} & e^{i\mathbf{k} \cdot \mathbf{r} + i\gamma \ln(kr - \mathbf{k} \cdot \mathbf{r})} [1 + O(1/r)] \\ & + f(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) \frac{e^{ikr - i\gamma \ln(2kr)}}{r} [1 + O(1/r)], \end{aligned} \quad (3)$$

where $f(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}})$ is the required scattering amplitude. Utilising surface-integral evaluation at some large r_0 one can show [14], for both short- and long-range potentials,

$$\langle \phi_{\mathbf{k}'} | \overleftarrow{H} - \epsilon | \psi_{\mathbf{k}}^+ \rangle_{r_0} = t(\mathbf{k}', \mathbf{k}), \quad (4)$$

which yields the required amplitude, and where $\phi_{\mathbf{k}'}$ is the analytically known asymptotic form of the incident-channel wavefunction.

The main idea is that in the surface-integral form, in which the potential of interaction disappears, at large r_0 , we are able to perform the integration with all quantities analytically known. The expressions given reduce to the usual ones in the case of short-range potentials.

The situation for the three-body problem relies on the same ideas, except that the asymptotic forms of three-body wavefunctions are more complicated. In the end, we have a definition for the amplitude and a practical method for its calculation for both the excitation and ionisation processes. The post form of the amplitude, Eq. (4) explains the success of the ECS and CCC methods in calculating ionization amplitudes. In the former, the asymptotic form of the total wavefunction is approximated by a product of two Coulomb waves, whereas in the CCC method the slow electron is represented by a Coulomb wave and the fast one by a plane wave. Further details may be obtained from Kadyrov *et al* [14].

3. Electron-impact total ionisation cross sections and spin asymmetries

Baum *et al* [15] measured, for Li, Na and K, the electron-impact total ionisation spin asymmetries A ,

$$A = \frac{\sigma_0 - \sigma_1}{\sigma_0 + 3\sigma_1}, \quad \sigma = \frac{1}{4}(\sigma_0 + 3\sigma_1), \quad (5)$$

where σ_S are the ionization cross sections, dependent on the total spin S , and σ is the total spin-averaged ionisation cross section. They noted that the K asymmetries were quite different to the other two and speculated on the cause. Using the CCC method [16] we have calculated the asymmetries, and present the results so as to explain the origin of the unexpected behaviour.

In figure 1 we give the results for Li. We see good agreement between CCC and experiment for the spin asymmetries from near threshold to the higher energies. The general shape is typical of the asymmetries, at threshold the asymmetry is around 0.5 indicating that the singlet cross section is around five times larger than the triplet one, and then they gradually diminish to zero ($\sigma_0 = \sigma_1$) with increasing energy. Looking at the individual σ_S we see the underlying behaviour of the cross sections that define the spin asymmetries. The cross sections rise from zero at threshold to some maximum and then slowly diminish with increasing energy. The shape of the asymmetries is determined by the relative rise from the threshold and the position of the maxima of the σ_S .

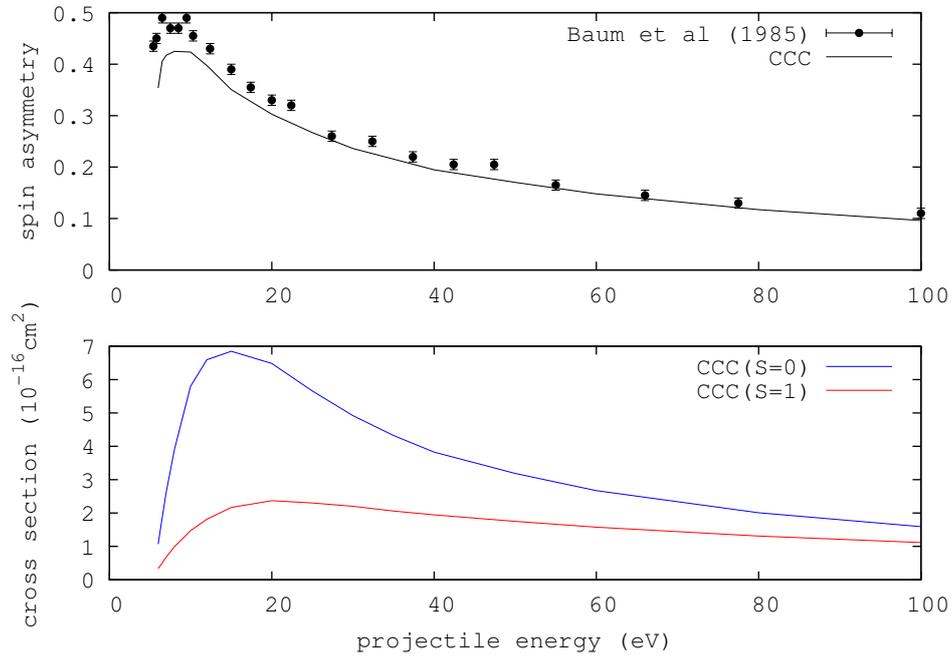


Figure 1. The e-Li total ionisation spin asymmetries and cross sections. The measurements are due to Baum *et al* [15]. The CCC calculations are due to Bray [17].

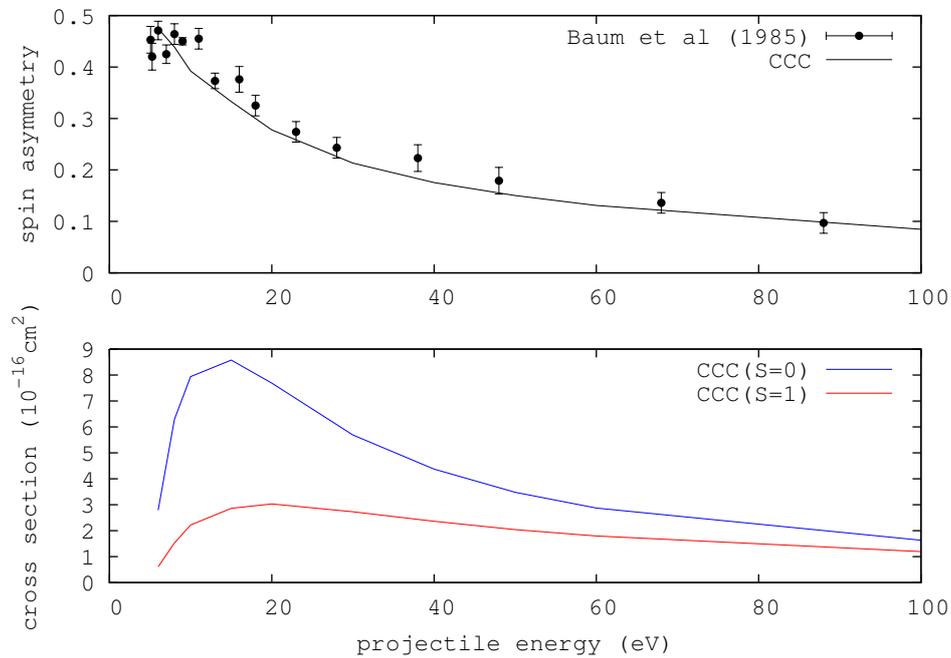


Figure 2. The e-Na total ionisation spin asymmetries and cross sections. The measurements are due to Baum *et al* [15]. The CCC calculations are due to Bray [12].

The Na case is considered in figure 2. This is quite similar to Li, for both the spin asymmetries and the magnitude of the cross sections σ_S .

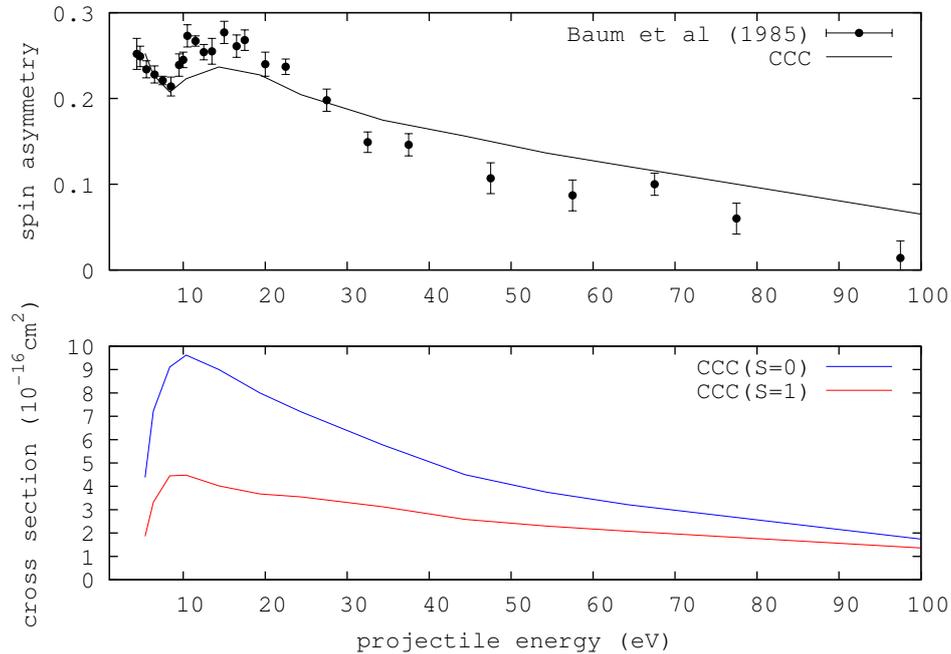


Figure 3. The e-K total ionisation spin asymmetries and cross sections. The measurements are due to Baum *et al* [15]. The present calculations are denoted by CCC.

However, the K case, given in figure 3, shows that the shape of the spin asymmetries has changed. Now there is a clear minimum around 9 eV, and yet there is little noticeable change in the qualitative behaviour in the corresponding σ_S . All that has happened is that the triplet cross section has increased a little in relative importance near threshold, and thereby reduced the spin asymmetry to around 0.25. The minimum observed is just due to the delicate interplay between the way the two cross sections rise, and is simply an indication of the sensitivity of ratio quantities such as spin asymmetries to the underlying absolute cross sections.

In figure 4 we consider the question of how do the spin asymmetries change if the target is a highly charged ion, specifically a Na-like ion Ar^{7+} . This question is interesting because we know that for highly charge ions the Coulomb-Born approximation yields reasonably accurate total ionization cross sections, but due to neglect of exchange yields identically zero spin asymmetries. We see that the CCC-calculated spin asymmetries have the same qualitative, and almost quantitative, behaviour as for Na, though now the ionisation threshold is much higher. Even though the Born approximation assumes that $\sigma_0 = \sigma_1$, which is clearly in substantial error over the entire energy range considered, the agreement for the total ionization cross section is remarkably good, particularly at energies above 400 eV. How can this be?

Agreement of Born plus exchange calculations with CCC suggests that coupling is negligible, and the cross sections can be obtained from the Born direct (D) and exchange (E) amplitudes. It then follows that these two amplitudes must satisfy $E^*E \approx \text{Re}(D^*E)$ over the energy range where the Born approximation is sufficiently accurate. Why this should be the case is currently under investigation.

4. Single and double photoionisation of lithium

We report the extension of the CCC formalism for single photon double ionisation (DPI) of two-electron targets (He and its isoelectronic sequence of ions [18], valence and K -shell DPI of alkaline-earth atoms [19, 20]) to three-electron targets (Li presently). In the CCC calculations,

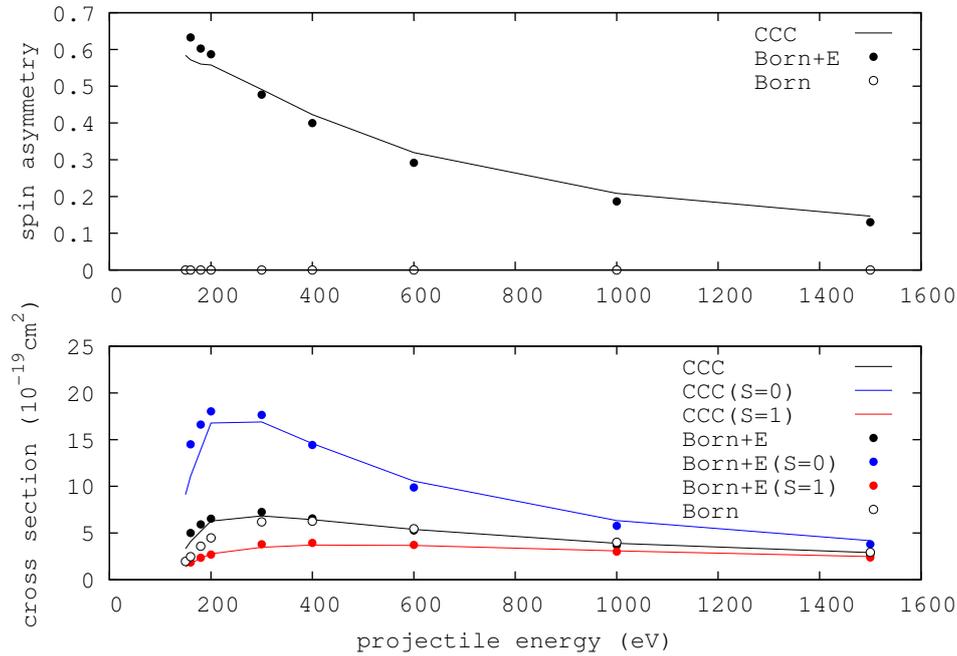


Figure 4. The e-Ar⁷⁺ total ionisation spin asymmetries and cross sections. The present convergent close-coupling calculations are denoted by CCC. The Coulomb-Born with Exchange approximation is labeled by Born+E. The pure Coulomb Born approximation is labeled by Born.

we treat DPI as a two step process. The first step is the full absorption of the photon energy by one electron. The second is electron impact ionisation of the singly charged ion which results in promotion of the remaining electron into the continuum. DPI calculations on two-electron targets requires CCC amplitudes of electron scattering on a singly charged hydrogenic target [16]. Similarly, DPI calculation on Li requires CCC amplitudes of electron scattering on a He-like Li⁺ ion [6].

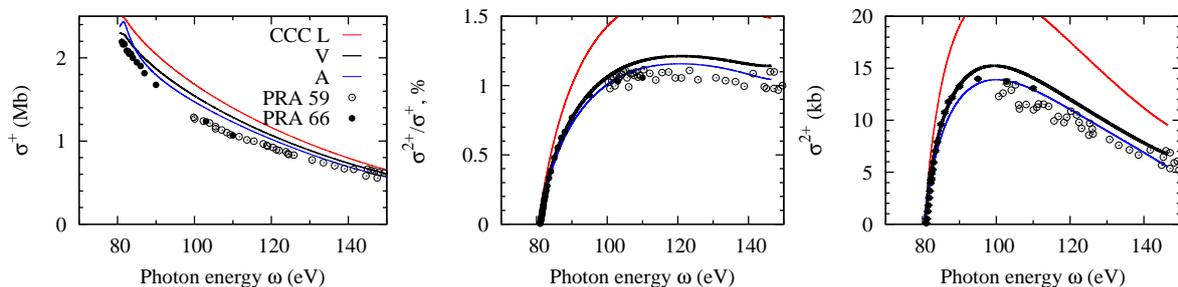


Figure 5. Photoionisation cross-sections of Li: single photoionisation σ^+ (left), double-to-single ratio σ^{2+}/σ^+ (center), DPI cross-section σ^{2+} (right). Experiments, labeled as PRA59 and PRA66, are from Refs. [21] and [22], respectively.

The total integrated cross-sections of single and double photoionisation of Li in the three gauges of the electromagnetic interaction (Length - L, Velocity- V and Acceleration - A) are presented in Figure 5 in comparison with experimental data. The L-gauge is unreliable for DPI calculations because of insufficient accuracy of the multi-configuration Hartree-Fock ground

state. However, the two other gauges are in good agreement with experiment. This is the first successful attempt to match these experimental data with an *ab initio* non-perturbative calculation. Earlier time-dependent close-coupling calculations [23] were restricted to higher photon energy range above the second DPI threshold at 152 eV.

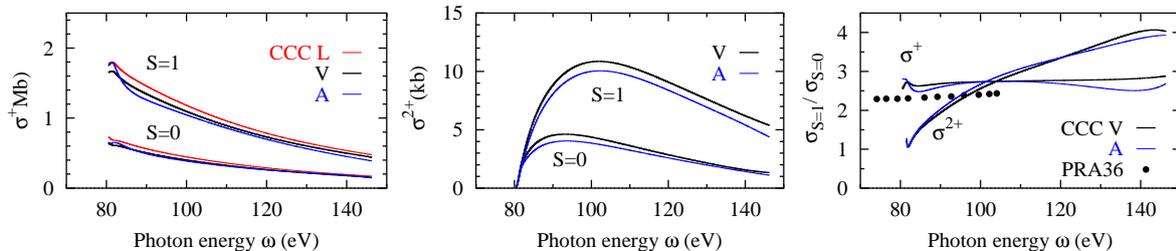


Figure 6. Spin-resolved photoionisation cross-sections of Li: single photoionisation σ^+ (left), DPI cross-section σ^{2+} (center), spin ratio $\sigma_{S=1}/\sigma_{S=0}$ (right). Earlier calculation of the spin ratio of single photoionisation reported in Ref. [24] is labeled as PRA36.

The first stage of DPI of Li can proceed via the singlet or triplet states $1s2s\ ^1,^3S$ of Li^+ . It was argued in Ref. [22] that the single photoionisation of the triplet state of Li^+ should be the dominant channel. This conclusion was based on scaling of the DPI of Li versus DPI of He with the respective ionisation potentials of the singly charged ion (1S or 3S in the case of Li^+). Our spin-resolved results shown in Figure 6 demonstrate this propensity explicitly. Predominant population of the singly ionised triplet state, with the spin ratio $\sigma_{S=1}^+/\sigma_{S=0}^+$ close to 3, is translated into the dominant triplet DPI channel. The spin ratio $\sigma_{S=1}^{2+}/\sigma_{S=0}^{2+}$ shows more noticeable variation with photon energy, decreasing near the threshold.

5. 64.6 eV electron-impact ionisation of helium

The CCC method has been very successful in reproducing the angle-differential measurements of electron-impact ionisation of helium [6, 9]. Following the work of Schulz *et al* [25] there has been an increased focus on out-of-plane geometries [26, 27]. The corresponding cross sections are generally a good deal smaller than the in-plane ones and we would expect that these would be correspondingly more difficult to measure and calculate.

In figure 7 we present a CCC calculation of 64.6 eV electron-impact ionisation of helium in the coplanar symmetric and perpendicular-plane geometries corresponding to the experiment of Murray and Read [28]. The data are available for four energy sharings of the 40 eV excess energy. At the equal-energy-sharing there are also the in-plane data taken in Kaiserslautern and reported by Bray *et al* [29]. Looking at the left panels, corresponding to the in-plane geometries, we see that there is a systematic discrepancy of CCC with the data [28] in the angular range of 30° to 60° , where the cross sections are the largest. However, in the perpendicular plane case, agreement is excellent over the entire angular range, though the magnitude of the cross sections is much smaller. Note that the maximum at 90° in the perpendicular geometry corresponds to almost a minimum in the in-plane case. This common point was used to normalise experiment to theory, separately for each energy-sharing. We are at a loss to explain these discrepancies. We note the considerably better agreement with the Kaiserslautern in-plane data, available only for equal energy-sharing, but how it is possible at the same time to obtain such excellent agreement for the very small out-of-plane cross sections is not a question we can answer. Performing CCC calculations of various basis sizes shows greatest variations in the smaller cross sections, as might be expected.

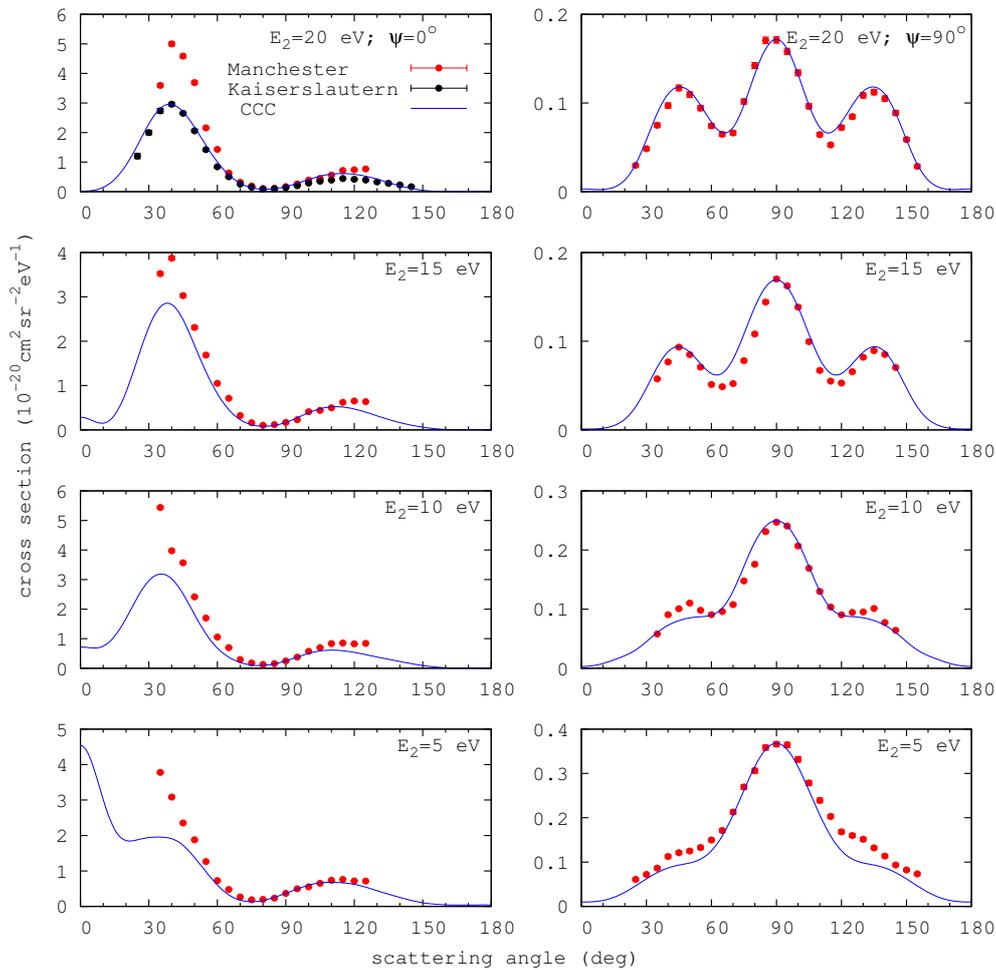


Figure 7. The 64.6 eV e-He fully differential ionisation cross sections for in-plane ($\psi = 0^\circ$) and out-of-plane ($\psi = 90^\circ$) incident electrons with outgoing electrons of energies E_2 and $40 - E_2$ measured in the symmetric ($\theta_1 = -\theta_2$) geometry. The present convergent close-coupling results are denoted by CCC. The Manchester and Kaiserslautern measurements are from refs.[28] and [29], respectively.

Acknowledgments

This work was supported by the Australian Research Council. We are grateful for access to the Australian National Computing Infrastructure Facility and its Western Australian node iVEC.

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