Electron-impact ionisation of atoms and ions

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Abstract. We report on the recent applications of the convergent close-coupling method to electron impact ionisation of atoms and ions. Total and fully differential cross sections are considered. Some excellent agreement with experiment is identified, but some long-standing discrepancies still remain.

Electron-impact ionisation of atoms and ions is of fundamental and practical interest. On the fundamental side, the interactions involve at least three charged particles. Such problems defied adequate formulation since the inception of Quantum Mechanics. Only very recently a workable formulation has been given [1]. On the practical side, ionisation cross sections are vital in modeling of artificial and astrophysical plasma processes. Electron-impact single ionisation cross sections range from the fully differential, where the energies and angles of the two outgoing electrons are specified, to the total, where all the angles and energy-sharings are integrated over. In this paper we review some recent applications of the convergent close-coupling (CCC) method to electron-impact ionisation. Note that the close-coupling method was originally intended for the calculation of excitation processes, thereby avoiding any issues associated with the boundary conditions in breakup problems with all charged particles. However, an extension of the CCC method to fully differential ionisation cross sections is particularly straightforward, see [2, 3, 4].

We begin by considering the e-Na ionisation problem. The sodium atom is treated as a one active electron above an inert Hartree-Fock core. A small polarisation potential is also added to take into account virtual core excitations. Such a treatment is sufficient to yield very accurate e-Na excitation cross sections [5]. Application to ionisation is a little problematic due to the possibility of ejecting a core electron, a significant contribution at sufficiently high energies. However, fully differential measurements ensure by energy conservation that it is the valence electron that is being ejected. Such measurements were performed by Murray [6] who measured the coplanar symmetric geometry for the case of equal energy outgoing electrons. Owing to the relatively small ionisation threshold of 5.1 eV, excitation of large angular momentum states becomes more probable, requiring some of the largest to date close-coupling calculations to obtain convergence. The details of the convergent close-coupling (CCC) calculations have been given by Bray et al [7], and the comparison with experiment is presented in figure 1.

The excellent agreement between the CCC theory and experiment for fully differential ionisation cross sections suggests that the same should hold for total ionisation cross sections. Indeed this is the case for atomic hydrogen, whether in the ground (1s) or excited (2s) state, see figure 2. In fact we are unaware of any significant discrepancies between CCC and experiment for any electron-impact ionisation processes. What the figure shows is that there is nothing
particularly special about the choice of the initial state, so long as convergence in the target states used to expand the total wavefunction is obtained.

The situation is not quite so simple if we consider helium, the next simplest target. In this case there is a substantial discrepancy between CCC and experiment, though only for the case where the initial state is \(2^3S\), see figure 3. This discrepancy is a long standing one with other similarly sophisticated theories in agreement with the CCC results [10].

Clearly, a new measurement of the e-He(\(2^3S\)) ionisation is desirable. While this has not yet happened a closely related measurement, that of electron impact ionisation of helium-like lithium (Li\(^+\)), has been performed for the ground state and a mix of the ground and metastable \(2^3S\) initial states [11]. The CCC theory for He is only marginally modified by the fact the the Li\(^+\) is a singly charged ion. If the theory can yield good agreement with measurements of e-Li\(^+\)(\(2^3S\)) ionisation then we can be even more confident in the corresponding He results.

By choosing different ways of creating Li\(^+\) Borovik et al [11] were able to control whether the target was prepared in a pure ground \(1^1S\) state, or a controlled mixture of the \(1^1S\) and \(2^3S\) states. Since the ionisation cross sections of the metastable states are much larger than for the ground state, and their thresholds are at much lower energies, their signal is unmistakable even for relatively small fractions in the target beam. In figure 4 we compare the experiment for the two cases with the CCC calculations. The left panel shows excellent agreement when the

Figure 1. Electron-impact on sodium fully differential equal energy-sharing ionisation cross section in the symmetric geometry. The experimental data and calculations are due to Murray [6] and Bray et al [7].
Figure 2. Electron-impact of atomic hydrogen total ionisation cross sections for the ground and 2s states. The measurements are due to Shah et al [8] and Dixon et al [9]. The calculations are due to Fursa and Bray [10].

beam contains pure Li$^+$ in the ground state. The right panel shows excellent agreement also, assuming that the beam contains around 13% of the metastable 2$^3S$ state. Such agreement over the broad energy range is only possible if the theory correctly obtains the cross sections for both initial states.

Figure 3. Electron-impact of helium total ionisation cross sections for the ground and 2$^3S$ states. The measurements are due to Shah et al [12] and Defrance et al [13]. The calculations are due to Bray and Stelbovics [14] and Bartschat and Bray [15].
Figure 4. Electron-impact ionisation of helium-like lithium in the ground and a mixture of the ground and $^{2}\SS$ states. The experiment and calculations have been recently presented by Borovik et al [11].

To conclude, the CCC theory has been shown to yield accurate fully differential ionisation cross sections for Na, a target more complicated than H or He. Application to e-Li$^{+}(2\SS)$ suggests that the CCC theory should also yield correct e-He($2\SS$) cross sections. Nevertheless, an independent experimental verification is still desirable.

Acknowledgments
This work was supported by the Australian Research Council and Curtin University. We are grateful for access to the Australian National Computational Infrastructure and its Western Australian node iVEC.

References
[1] Kadyrov A S, Bray I, Mukhamedzhanov A M and Stelbovics A T 2008 Phys. Rev. Lett. 101 230405 (pages 4)
[2] Bray I and Fursa D V 1996 Phys. Rev. A 54 2991–3004
[3] Bray I 2002 Phys. Rev. Lett. 89 273201
[4] Stelbovics A T, Bray I, Fursa D V and Bartschat K 2005 Phys. Rev. A 71 052716(13)
[5] Bray I 1994 Phys. Rev. A 49 1066–1082
[6] Murray A J 2005 Phys. Rev. A 72 062711
[7] Bray I, Fursa D V and Stelbovics A T 2008 J. Phys. B 41 215203
[8] Shah M B, Elliot D S and Gilbody H B 1987 J. Phys. B 20 3501–3514
[9] Dixon A J, Harrison M F A and Smith A C H 1976 J. Phys. B 9 2617–2631
[10] Fursa D V and Bray I 2003 J. Phys. B 36 1663
[11] Borovik Jr A, Müller A, Schippers S, Bray I and Fursa D V 2009 J. Phys. B 42 025203 (10pp)
[12] Shah M B, Elliot D S, McCallion P and Gilbody H B 1988 J. Phys. B 21 2751–2761
[13] Defrance P, Claey s W, Cornet A and Poulaert G 1981 J. Phys. B 14 111–117
[14] Bray I and Stelbovics A T 1993 Phys. Rev. Lett. 70 746–749
[15] Bartschat K and Bray I 1996 J. Phys. B 29 L577–L583