Atomic photoionisation calculated using the singularity-free convergent close-coupling method

A. W. Bray[*1], **A. S. Kheifets**[*2], **I. Bray**[†3]

[*] Research School of Physics and Engineering, Australian National University, Canberra ACT 2601, Australia
[†] Department of Physics, Astronomy and Medical Radiation Science, Curtin University, WA 6845 Perth, Australia

Synopsis The coupled equations in the convergent close-coupling method have recently been solved by treating the singular Green's function analytically. We show that this is particularly advantageous in the case of calculating atomic single photoionisation with excitation near, and at the thresholds.

The convergent close-coupling (CCC) method [1] was initially developed for electron scattering on atomic hydrogen. It was then extended to ionic targets [2], which allowed it to be applied to calculating photoionisation of helium [3]. The basic idea is that the final state is constructed from the CCC calculation of e-He^+ scattering. Excitation of the negative-energy He^+ states is associated with single photoionisation with excitation. Excitation of the positive-energy states is associated with double photoionisation.

The CCC method solves the coupled equation in momentum space, which contains a singular Green's function requiring a principal value integration over the projectile virtual momentum. The numerical implementation of this integration is problematic in the near threshold regions where the singularity approaches zero. To address this problem a new numerical implementation takes the integral analytically for neutral [4, 5] and charged targets [6]. This allows the results to be obtained accurately not only in the near threshold regions, but also explicitly at thresholds.

We demonstrate this in the figure by the application to single photoionisation of helium with $n \leq 3$ excitation, from thresholds to high energies. Two sets of CCC calculations are presented, the original and the new. The latter approach is also able to be applied by setting the energy to be the exact threshold of interest, and these results are denoted by the arrows. For completeness, the double photoionisation cross section is also presented.

The differences between the two numerical implementations of the CCC method are evident only in the near threshold region, which has been exagerated by using a logarithmic energy scale. Clearly the singularity-free one is superior, and the fact that it is able to be applied at exact thresholds provides extra utility to the new approach.

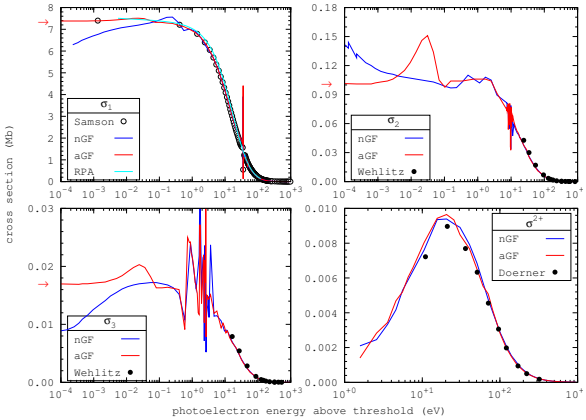

Figure 1. phoionisation of helium cross sections with excitation to $n \leq 3$ states calculated using the new singularity-free CCC method (red), and the original CCC method (blue). The red arrows indicate the result when the new method is applied exactly at threshold. For completeness, the double photoionisation cross section is also presented.

References

[1] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).

[2] I. Bray, Phys. Rev. A **49**, 1066 (1994).

[3] A. S. Kheifets and I. Bray, Phys. Rev. A **58**, 4501 (1998).

[4] A. W. Bray, I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, and I. Bray, Comp. Phys. Comm. **196**, 276 (2015).

[5] A. W. Bray, I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, and I. Bray, Comp. Phys. Comm. **203**, 147 (2016).

[6] A. Bray, I. Abdurakhmanov, A. Kadyrov, D. Fursa, and I. Bray, Computer Physics Communications **212**, 55 (2017).

[1]E-mail: Alexander.Bray@anu.edu.au
[2]E-mail: Anatoli.Kheifets@anu.edu.au
[3]E-mail: Igor.Bray@curtin.edu.au