Various problems in electron-atom collision theory

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Abstract. We outline progress in a broad range of research projects that are currently being undertaken in our group. These include the formulation of ionisation amplitudes in Coulomb few-body problems, a new convergent close-coupling implementation for electron-helium collisions, elastic electron-magnesium scattering at very low energies, and the calculation of electron-cesium spin asymmetries and differential cross sections.

INTRODUCTION

The field of electron-atom collision theory is progressing at a rapid pace. Ever-growing modern computational facilities are allowing for the study of more and more complicated collision systems. Our primary motivation in developing a general computer code, the convergent close-coupling (CCC) method for electron/positron/photon collisions with atoms, is driven by applications. Such collision data are necessary to understand astrophysical and laboratory plasmas, and they are of crucial importance in the research and development of new lighting sources.

The interaction with experiment is as crucial as ever. Though much theoretical progress has been made in the treatment of relatively simple quasi-one- and quasi-two-electron atomic targets, the same cannot be said for heavier and more complicated systems. In these cases approximate treatments of the multitude of relatively inactive target electrons are necessary, and the accuracy of such approximations must be thoroughly tested not only by investigating structure issues, but also by comparison with the results from collision studies. We use data from highly detailed and sophisticated experiments to test the theoretical method, expecting the results to be subsequently used with considerable confidence in modelling applications.

FORMAL IONISATION THEORY

The success of the exterior complex scaling (ECS) [1, 2] and CCC [3] methods for ionisation requires some investigation given the uncertain status of formal ionisation

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theory. Peterkop's [4] formulation suffers from the fact that the phase of the ionisation amplitude cannot be uniquely defined, yet a formal solution of the problem must yield a unique amplitude of a specified magnitude and phase. Accordingly these issues have been carefully reanalysed by Kadyrov et al. [5] and Kadyrov et al. [6]. Briefly, the correct boundary conditions for all kinematical arrangements leading to ionisation have been determined. Ionisation amplitudes may now be defined unambiguously and related to those given by Peterkop [4] and the ECS theory [2]. As a consequence, an explanation is given for why the ECS theory yielded accurate cross sections, but with the underlying phases showing rapid oscillation as a function of the hyper-radius R. Furthermore, a relation exists that eliminates such oscillations and yields the true phase [7]. How such considerations affect further application of the CCC approach to ionisation is yet to be determined.

BOX-BASED CCC APPROACH TO ELECTRON-HELIUM COLLISIONS

The box-based CCC approach (CCC-B) was first implemented for the atomic hydrogen target [8] and then extended to helium [9]. The idea is simply to replace the Laguerre basis in the original CCC method (CCC-L) with eigenstates obtained by solving a one-electron Schrödinger equation in a box of size R_0. In the case of helium the one-electron orbitals are obtained by solving such an equation for the He^+ ion. These are then used to construct two-electron configurations and the calculations proceed as originally outlined by Fursa and Bray [10].

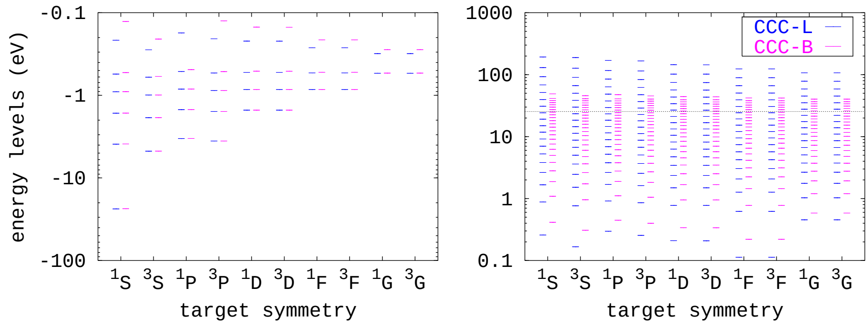

FIGURE 1. Energy levels in the CCC-L (left) and CCC-B (right) calculations. For 50 eV e-He collisions, states above the total energy line at 25.4 eV are closed.

To demonstrate how the e-He CCC-B method works and to contrast it to the CCC-L method we take $R_0 = 50$ a.u. for CCC-B, and $N_l = 29 - l$ with $\lambda_l = 2.2$ in the Laguerre basis of the CCC-L calculation. In Fig. 1 we present a comparison between the helium energy levels arising in the CCC-B and CCC-L calculations of 50 eV e-He scattering. The lower energy states are quite similar in their distribution, but as the energies increase the CCC-B spectrum become much more dense. Even though the CCC-L states extend higher in energy there are in fact more CCC-B states in the figure.

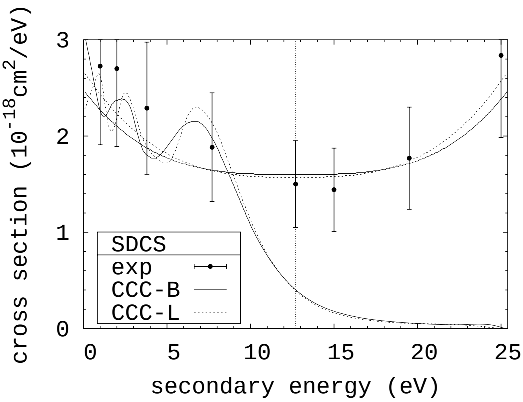

FIGURE 2. Singly differential cross sections obtained in the CCC-L and CCC-B calculations for 50 eV e-He ionisation. The symmetric (around 12.7 eV) results are estimates based upon the step-function behaviour of the raw CCC results (see text). Experiment is due to Röder et al. [12].

Having defined the target structure we proceed in the usual way [10] to calculate the scattering amplitudes from the ground state to each of the open states. The amplitudes for excitation of the positive-energy states are then used to define the ionisation amplitudes [11]. From these, in turn, the various ionisation cross sections are generated.

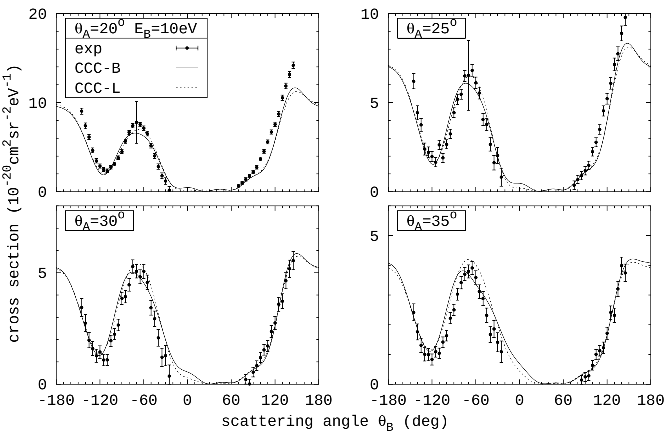

FIGURE 3. Triply (fully) differential cross sections obtained in the CCC-L and CCC-B calculations for 50 eV e-He ionisation with the 10 eV electron detector fixed at the specified angles θ_A. Experiment is due to Röder et al. [12].

We begin with the singly differential cross section (SDCS), exhibited in Fig. 2. The raw CCC results show remarkable similarity, particularly in the region above the equal-energy point of $E/2 = 12.7$ eV, where there are many more CCC-B than CCC-L states (c.f. Fig. 1). The oscillations are expected as an explicitly antisymmetrised close-coupling expansion appears to behave like a Fourier expansion of the underlying step-function amplitudes [13]. The symmetric (around $E/2$) SDCS are obtained from an integral-preserving estimate with the SDCS at $E/2$ being four times the raw result. (The amplitude at the step is half the step height.)

Having examined the SDCS, we turn to the triply differential cross sections (TDCS) measured with the $E_B = 10$ eV detector rotated in the plane and the $E_A = 14.7$ eV detector fixed at the specified angles. These kinematics are particularly interesting for us because the raw SDCS results are well below the estimated true predictions at this energy. The available measured TDCS are compared with the CCC results in Fig. 3. The presented CCC-calculated TDCS have been scaled to ensure that the estimated SDCS is obtained upon angular integration. Such a procedure does not affect the angular profiles, but it brings about excellent absolute agreement with the experiment.

LOW-ENERGY ELECTRON-MAGNESIUM ELASTIC SCATTERING

This problem has been recently examined by Bartschat and Sadeghpour [14] and by Gedeon et al. [15] using R-matrix methods. However, when attempting to verify their results using the CCC method, we found unexpected difficulties in obtaining convergent results. An example is given in Fig. 4. In this work 150-state close-coupling calculations were performed with the Laguerre exponential fall-off parameter slightly varied around $\lambda = 4$. The 150 states arose upon taking five s- and five p-orbitals of a Laguerre basis and allowing for all possible resulting configurations.

Starting with the $L = 0$ partial wave, we see an enormous variation of the results as a function of λ. At the time of writing this manuscript, we could not conclusively determine either the cross section or even the sign of the scattering length. As λ increases, the positive phase-shift for $\lambda = 3.6$ monotonically decreases and goes through zero, as does the cross section, around $\lambda = 4.0$.

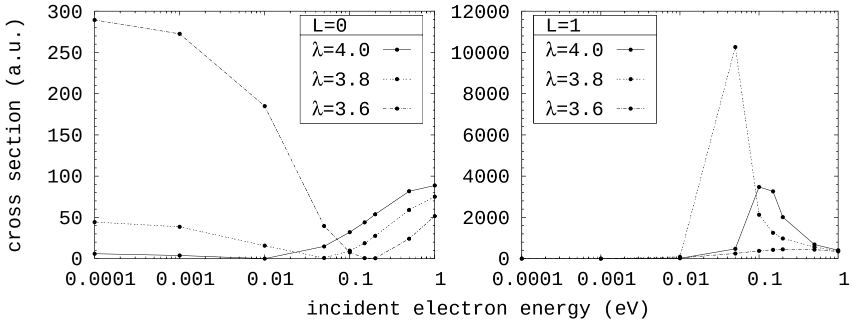

FIGURE 4. Elastic partial cross section for e-Mg scattering obtained in a 150-state close-coupling model (see text).

The $L = 1$ partial wave is just as interesting. Here Burrow et al. [16] identified a shape-resonance around 0.16 eV. This is consistent with the $\lambda = 4.0$ calculation and the results from the R-matrix calculations mentioned above. However, as λ is reduced, the resonance position is shifted to lower energies, leading to a rapid rise in the cross section, and then pushed even to negative energies implying a bound state and a collapse in the cross section. Clearly much larger CCC calculations are necessary to establish convergence for both partial waves.

SPIN-ASYMMETRIES AND DIFFERENTIAL CROSS SECTIONS IN ELECTRON-CESIUM COLLISIONS

Spin-resolved measurements provide some of the most thorough testing ground of atomic collision theory. One of the major verifications of the accuracy of the CCC approach was obtained by application to such data available for the electron-sodium system [17]. The electron-cesium collision problem is somewhat similar, except that the target structure is more difficult and relativistic effects may be important [18, 19]. One major difference between the Na and Cs targets is the much larger core dipole polarisation α_d of Cs^+ $(15.6\,a_0^3)$ compared to Na^+ $(1.0\,a_0^3)$. Accordingly, the effect of α_d on the scattering process is small for the e-Na system, but we check it here for the e-Cs elastic scattering and 5d-excitation.

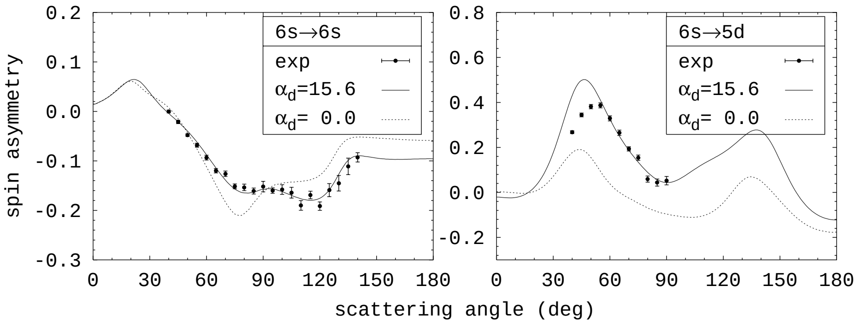

FIGURE 5. Spin asymmetries for 8 eV e-Cs elastic scattering (6s→6s) and 6s→5d excitation. The experimental data are from Baum et al. [18, and private communication].

As an example, we consider the case of 8 eV incident electrons. The CCC calculations yield convergence very easily for the parameters considered by just taking 39 states with $l_\mathrm{max} = 3$. We found that treatment of the target continuum was just as important here as it was for sodium [17]. In Fig. 5 we present spin-asymmetries for the two transitions studied and see that α_d significantly affects the results, with the correct value yielding excellent agreement with experiment. In Fig. 6 we then compare preliminary measurements for the relative DCS with the CCC predictions. While agreement with the elastic DCS improves with the correct value of α_d, this is not so for 5d-excitation. A reexamination of the phenomenological dipole core-polarisation treatment may therefore be required.

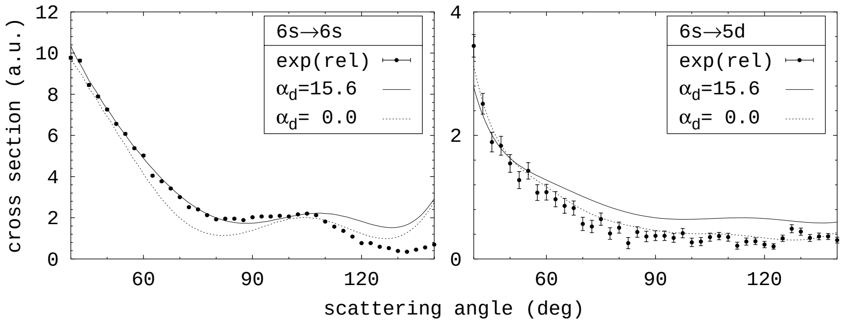

FIGURE 6. Differential cross sections for 8 eV e-Cs elastic scattering and 6s→5d excitation. The CCC calculations are described in the text. The experiment is as for Fig. 5.

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REFERENCES

1. Rescigno, T. N., Baertschy, M., Isaacs, W. A., and McCurdy, C. W., *Science*, **286**, 2474–2479 (1999).
2. Baertschy, M., Rescigno, T. N., and McCurdy, C. W., *Phys. Rev. A*, **64**, 022709 (2001).
3. Bray, I., Fursa, D. V., Kheifets, A. S., and Stelbovics, A. T., *J. Phys. B*, **35**, R117–R146 (2002).
4. Peterkop, R. K., *Theory of Ionization of Atoms by Electron Impact*, Colorado Associated University Press, Boulder, 1977.
5. Kadyrov, A. S., Mukhamedzhanov, A. M., and Stelbovics, A. T., *Phys. Rev. A*, **67**, 024702 (2003).
6. Kadyrov, A. S., Mukhamedzhanov, A. M., Stelbovics, A. T., Bray, I., and Pirlepesov, F., *Phys. Rev. A*, **68**, 022703 (2003).
7. Kadyrov, A. S., Mukhamedzhanov, A. M., Stelbovics, A. T., and Bray, I., *Phys. Rev. Lett.*, submitted (2003).
8. Bray, I., Bartschat, K., and Stelbovics, A. T., *Phys. Rev. A*, **67**, 060704(R) (2003).
9. Bray, I., Bartschat, K., Fursa, D. V., and Stelbovics, A. T., *J. Phys. B*, **36**, 3433–3455 (2003).
10. Fursa, D. V., and Bray, I., *Phys. Rev. A*, **52**, 1279–1298 (1995).
11. Bray, I., and Fursa, D. V., *Phys. Rev. A*, **54**, 2991–3004 (1996).
12. Röder, J., Ehrhardt, H., Bray, I., Fursa, D. V., and McCarthy, I. E., *J. Phys. B*, **29**, L67–L73 (1996).
13. Stelbovics, A. T., *Phys. Rev. Lett.*, **83**, 1570–1573 (1999).
14. Bartschat, K., and Sadeghpour, H. R., *J. Phys. B*, **36**, L9–L15 (2003).
15. Gedeon, V., Lengyel, V., Zatsarinny, O., and Kocher, C. A., *Phys. Rev. A*, **59**, 2016–2029 (1999).
16. Burrow, P. D., Michejda, J. A., and Comer, J., *J. Phys. B*, **9**, 3225–3236 (1976).
17. Bray, I., *Phys. Rev. A*, **49**, 1066–1082 (1994).
18. Baum, G., Pavlovič, N., Roth, B., Bartschat, K., Fang, Y., and Bray, I., *Phys. Rev. A*, **66**, 022705 (2002).
19. Andersen, N., and Bartschat, K., *J. Phys. B*, **35**, 4507–4525 (2002).