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Close-coupling calculations of 64.6 eV e-He ionization

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Abstract. The convergent close-coupling and the time-dependent close-coupling methods are applied to the calculation of 64.6 eV electron-impact ionization of the ground state of helium resulting in two 20 eV outgoing electrons. The results of the calculations are compared with measured fully differential cross sections in various geometries. For the generally large in-plane geometries there is good agreement between the two theories and experiment. For the out-of-plane case the cross sections are generally smaller and some differences between the two calculations are evident, as well as experiment.

1. Introduction

The problem of calculating fully differential electron-impact ionization cross sections has seen enormous progress in the last decade. The goal of yielding accurate cross sections irrespective of geometry or kinematics can only be attained by non-perturbative approaches that aim to numerically solve the full few-body problem. The exterior complex scaling method of Rescigno *et al* [1, 2] was first to show that this was indeed possible for the e-H ionization problem. This was followed soon after by the convergent close coupling (CCC) method [3], and the time-dependent close-coupling approach [4]. It is our view that these techniques are able to fully solve the e-H three-body problem by providing results of sufficiently high accuracy for comparison with experiment.

The e-He problem is a four-body problem and may be expected to be substantially more difficult than the e-H system. Due to the tight binding of the He^+ electron, the He discrete spectrum consists of only one-electron excitations. Hence, the e-He interactions are dominated by one-electron transitions. This allows the reduction of the e-He four-body problem to essentially a three-body problem, not much more difficult than the e-H system. The CCC approach typically treats e-He in the frozen-core approximation, that keeps one electron in the ground state of He^+. This can be relaxed, if necessary, to use a multi-configuration treatment of He, but this has been found only necessary for more complex targets such as Mg. Sufficiently good agreement with e-He experiments of the frozen-core model is a reflection of the quality of the approximation. It has to be noted that the e-He system also has ionization plus excitation, and double ionization processes. These are much smaller in magnitude than the one-electron processes, and remain a formidable challenge to theory, see Pindzola *et al* [5] for example.

Electron scattering on helium is one of the most experimentally studied collision problems in atomic physics. The determination of (often) absolute fully differential cross sections for one-electron ionization by, in particular, the Kaiserslautern and Manchester groups over two decades [6]-[17] has given an excellent foundation for the testing of theory. So much so that we wonder whether the e-He single ionization problem can also be regarded as solved in the same way as the e-H system. The purpose of this article is to briefly address this issue.

2. Theory

We shall present the results of two non-perturbative approaches to the problem of calculating one-electron ionization of helium by electron impact. The specific problem we consider is 64.6 eV electron-impact ionization of helium with two 20 eV outgoing electrons, leaving the He^+ ion in the ground state.

2.1. Convergent close-coupling (CCC) method

The CCC method for the general e-He collision problem [18] expands the total wavefunction using states obtained by diagonalizing the target Hamiltonian in a two-electron Laguerre basis. In the frozen-core approximation one of the electrons is restricted to be the 1s orbital of He^+. This generally suffices for scattering from the He ground state, but a multi-configuration treatment may be required when scattering from the helium metastable states or more complex two-electron targets, see Refs. [19, 20] for example. The expansion states have negative- and positive-energy states relative to the ground state energy of He^+ (-54.4eV). With increasing basis size the negative-energy states yield an increasing number of He discrete eigenstates, and the positive-energy states provide an increasingly dense discretization of the He one-electron continuum. Solution of the resulting close-coupling equations is performed in momentum space yielding scattering amplitudes for all open states. Ionization is associated with excitation of the positive-energy states.

The extension of the CCC method to generate the ionization scattering amplitudes has proved to be remarkably simple [21], though it took some time to fully appreciate the consequences. Briefly, the scattering amplitude for a positive energy state is multiplied by the overlap of the state and the corresponding true continuum state of the same energy. The origin of this treatment has only been fully understood following the derivation of the expression necessary to calculate true ionization scattering amplitudes [22, 23]. Furthermore, as the availability of the computational resources continued to grow it was realized that the underlying scattering amplitudes exhibited step-function behaviour, with the step being at the equal-energy sharing point [24]. At that point the ionization amplitudes can always be obtained ab initio from coherent combinations of the underlying amplitudes for both hydrogen [25] and helium [26]. It is the latter formulation that we use here.

2.2. Time-dependent close-coupling (TDCC) method

The TDCC method as applied to the electron-impact single ionization of helium has previously been described in some detail [27, 28]. Briefly, an expansion of the total electronic wavefunction for the two outgoing electrons in products of radial functions and coupled spherical harmonics is used to express the Schrödinger equation in terms of a set of time-dependent coupled partial differential equations.. The non-ionized electron of helium is frozen and its interaction with the two outgoing electrons is represented through direct and local exchange potential terms. The interaction between the two outgoing electrons is treated in full. The time-dependent equations are propagated for each LS (total orbital angular and spin angular momentum, respectively), for sufficient L so that the resulting triple differential cross sections are completely converged. In the equal-energy calculations presented here, it was found that the TDCS was well converged with around 10 L contributions, although for asymmetric energy sharings, more terms are usually needed.

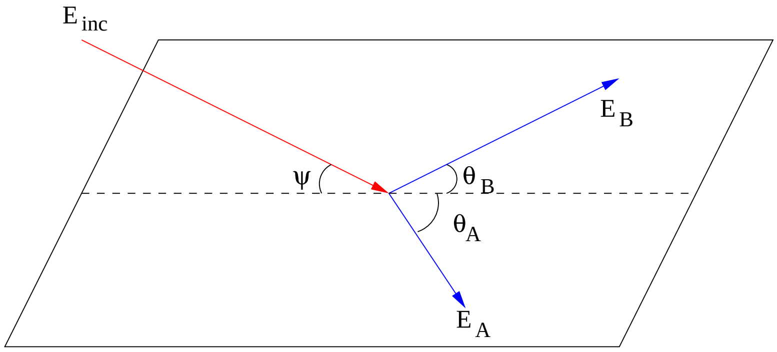

Figure 1. Orientation of detectors in an (e,2e) experiment, for coplanar ($\psi = 0°$), and out-of-plane geometries.

3. Results

A convenient way to parametrize the (e,2e) geometries is given in figure 1. The angle of the incident beam to the scattering plane is ψ. For example, in the coplanar case $\psi = 0°$, and in the perpendicular-plane case $\psi = 90°$. We use negative and positive angles to indicate detectors

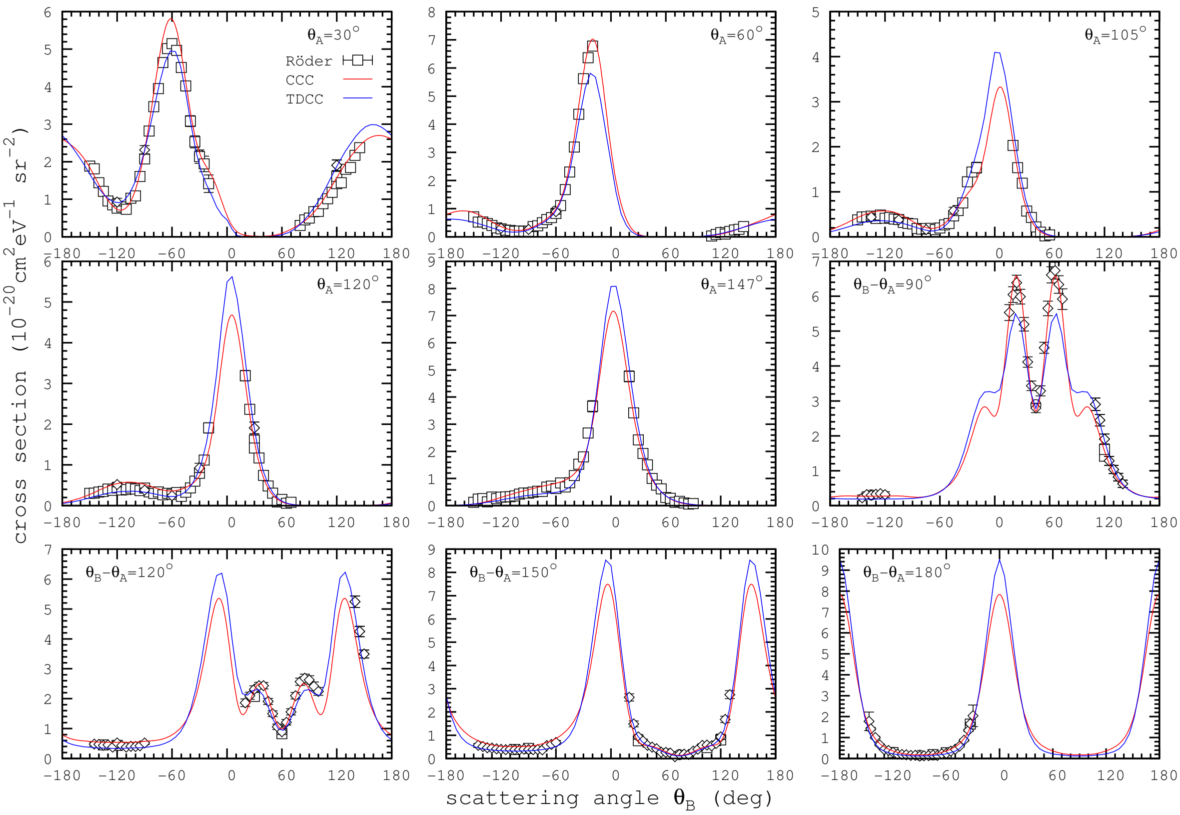

Figure 2. (Colour online) Fully differential cross sections for 64.6 eV electron-impact coplanar ionization of the ground state of helium with two 20 eV outgoing electrons. The data of Röder [29] have absolute uncertainty of 25% and have been multiplied by 1.2 for overall best visual fit to the theory.

on opposite sides to the incident beam.

In figure 2 we consider the coplanar case measured by Röder, and first presented by Bray *et al* [29]. The measurements are given with statistical uncertainty of around 5% and an absolute uncertainty of 25%. To enable best visual comparison between theory and experiment the latter have been uniformly multiplied by 1.2, which is well within the experimental uncertainty. Two types of geometries are being considered. One has a detector fixed at θ_A and the other is rotated in the plane from $-180°$ to $180°$, where possible. Such geometries show the typical behaviour of a dominant binary peak and and a smaller recoil peak. The other geometry has the angular separation of the two detectors $\theta_B - \theta_A$ fixed, which are then rotated together. These geometries readily show how electron-electron repulsion drops the cross sections as this angle is reduced.

We see that the agreement between the results of the two theories and experiment is remarkable for all cases considered. Seeing such a spectacular agreement it would be tempting to suggest that the e-He problem may well be solved.

In figure 3 we present the out-of-plane cross sections measured by Murray and Read [15]. The geometries are such that the incident electron is at the angle ψ to the plane containing the two detectors at symmetric angles on the opposite side of the incident beam. The $\psi = 0°$ case is the so-called coplanar doubly symmetric geometry, has also been measured by Röder [29]. One interesting aspect of these geometries is that for all values of $0° \leq \psi \leq 90°$ the $\theta_B = -\theta_A = 90°$ point is common. This seems an ideal point of normalization since the data of Murray and Read [15] were not independently normalized.

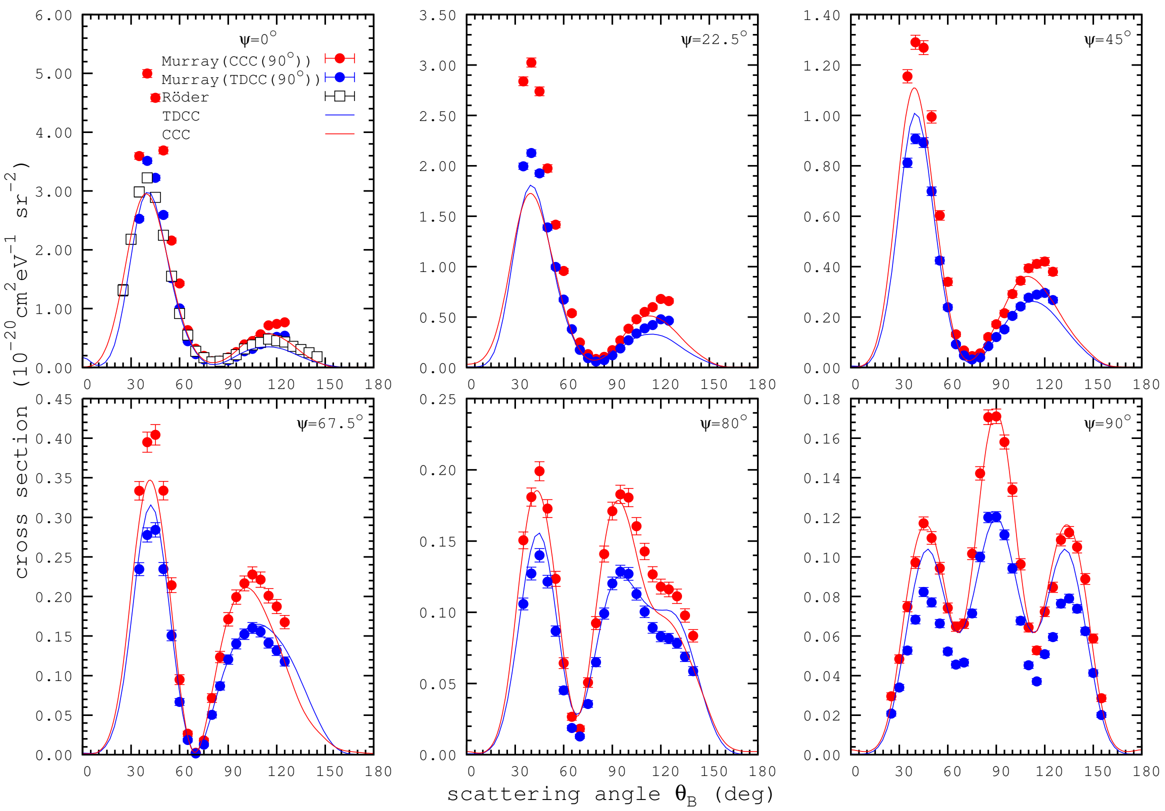

Figure 3. (Colour online) Fully differential cross sections for 64.6 eV electron-impact out-of-plane ionization of the ground state of helium with two 20 eV outgoing electrons. The data of Murray and Read [15] are presented twice: once normalized to the CCC(90°) point and again to the TDCC(90°) point. The data of Röder [29] is as for figure 2.

Though the $\theta_B = 90°$ point is common, its value is near the minimum of the $\psi = 0°$ geometry, and yet a maximum for the perpendicular-plane $\psi = 90°$ geometry. To make things more complicated, the two theories differ substantially in their predictions for the cross section at this point. Accordingly we have chosen to present the data normalized in two ways: once to the CCC(90°) point and also to the TDCC(90°) point.

Starting at the $\psi = 0°$ case we see the largest cross sections, and the normalization to TDCC(90°) yields best agreement with the data of Röder [29]. The theories are in good agreement with each other and the experimental data. The same holds for $\psi = 22.5°$ and $\psi = 45°$ cases. However, as ψ increases further we see that the discrepancy between the CCC and TDCC theory begins to grow with the shape of the data being unable to differentiate as to which theory may be the more accurate. The exception to that is the $\psi = 90°$ case where the CCC result yields remarkable shape-agreement with the data. This may be a coincidence as normalization here leads to a major discrepancy for the largest cross sections when $\psi = 0°$.

4. Conclusions

We have presented the results of the CCC and TDCC calculations for 64.6 eV electron-impact single ionization of the ground state of helium yielding two 20 eV outgoing electrons. The difference between the results of the two calculations are only evident when the cross sections are particularly small. Existing measurements are in sufficiently good agreement with the theory so as to be unable to differentiate between them. In order for that to be possible, new measurements are required. For example, obtaining the ratio of the cross sections at the 90° point of figure 3 and say the 45° point of the $\psi = 0°$ geometry would be very helpful. We are hopeful that the measurements currently underway will be able to differentiate between the CCC and TDCC theories for the presently considered equal energy sharing case, and also for asymmetric energy sharing [30].

Acknowledgments

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