Electron-impact ionization of helium with large energy transfer

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We consider the recently measured case of 730 eV electron-impact ionization of the ground state of helium with 205 and 500 eV coplanar outgoing electrons by Catoire *et al.* [J. Phys. B **39**, 2827 (2006)]. These measurements, which are on a relative scale, show some unexpected structure and variation from the second-order distorted-wave Born approximation *R*-matrix and Brauner-Briggs-Klar theories. Using the convergent close-coupling method we provide an improved agreement with experiment, but some discrepancies still remain.

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There has been much progress in the field of theoretical description of electron-impact ionization of simple atoms such as hydrogen and helium. This has come predominantly from nonperturbative approaches such as exterior complex scaling (ECS) [1–3], time-dependent close-coupling (TDCC) [4,5] and the convergent close-coupling (CCC) [6–8]. Given the success of the earlier application of distorted-wave methods at high energies with highly asymmetric kinematics, see for example [9] and references therein, much of the investigation in recent times has centered on the lower incident energies. The case of high energy incident electrons with two fast outgoing electrons has been relatively neglected.

Recently, Catoire *et al.* [10] measured coplanar triply differential cross sections (TDCS) for 730 eV electrons ionizing the ground state of helium with the two outgoing electrons having unusually high energies of 205 and 500 eV. The data, presented for the fixed angles of the fast electron at 3, 6, and 9°, were neither normalized nor internormalized, but did show some unexpected behavior at some of the scattering angles of the slower electron. The data was compared with various distorted-wave (DWBA) based calculations and another based on the boundary condition formalism (BBK) of Brauner, Briggs, and Klar [11]. All calculations reproduced the qualitative behavior of a dominant binary maximum, but showed considerable variation with experiment and with each other at scattering angles away from the maximum, where the DWBA yielded better qualitative agreement with the experiment. Additionally, there was some variation in the theories regarding the absolute values. We apply the CCC method to this problem in order to provide what we believe to be accurate absolute values and address the remaining qualitative discrepancies between theory and experiment.

The CCC method has been extensively applied to the problem of calculating fully differential electron-impact ionization cross sections. It is based on solving the close-coupling equations in momentum space [12], with ionization associated with excitation of the positive-energy pseudostates. The ability of the theory to reproduce total electron-impact ionization cross sections for hydrogen [13] and helium [14] gave us the confidence to apply the method to calculate fully differential cross sections [6]. The strength of the CCC method is that convergence in the cross sections of interest may be systematically checked by simply increasing the basis size. This is due to the fact that the target expansion states are obtained by diagonalizing the target Hamiltonian in an orthogonal Laguerre basis. As a consequence the CCC theory may be applied from low to high energies, where for the latter it converges naturally to the Born approximation. Additionally, as with other theories, we can check the convergence with respect to partial-wave expansions, the quality of the ground state, and the importance of incorporating electron-electron exchange.

For the present kinematics, where we have a relatively large incident energy, the Born approximation is going to be quite accurate for most of the discrete singlet excitation channels and ionization for the most asymmetric ($E_B \ll E_A$) kinematics. On the other hand, if we were interested in ionization with equal-energy ($E_A = E_B \approx 350$ eV) outgoing electrons then exchange would be critically important. Therefore, one question worth answering is whether exchange is important for the specific case of $E_B = 205$ eV and $E_A = 500$ eV. By performing calculations with and without exchange we found the results unaltered and so conclude that here exchange is not important. A second question is whether the frozen-core approximation, that has been so successful in describing *e*-He collisions generally, is still sufficiently accurate for the case of interest here. The biggest error in the frozen-core approximation is that for the ground state binding energy. This leads to an ionization threshold error of 0.84 eV. We can substantially improve the ground state by relaxing the frozen-core approximation and see the effect on our results as we do so. Once again, we found that such a variation leads to a negligible effect on the results and we conclude that the frozen-core approximation remains sufficiently accurate.

The CCC calculations are characterized by the maximum orbital angular momentum ($l_{\max}$) of the target expansion states, and the number of states N_l for each $0 \leqslant l \leqslant l_{\max}$. With the slow electron (described by the 205 eV pseudostates) having a relatively high energy, we need to ensure that $l_{\max}$ is sufficiently large. Since the CCC method is unitary, there is relatively little probability of exciting the larger l pseudostates. The major contribution to the TDCS comes from $l=1$, and we find that $l_{\max}=5$ is sufficient for convergence. By taking $N_l = 25 - l$ we also find sufficient convergence in the cross sections of interest. The total number of partial waves treated is effectively infinite through the usage of the analytic Born approximation to compute the contribution of the higher partial waves (>30 presently).

We first check the accuracy of the calculated total ioniza-

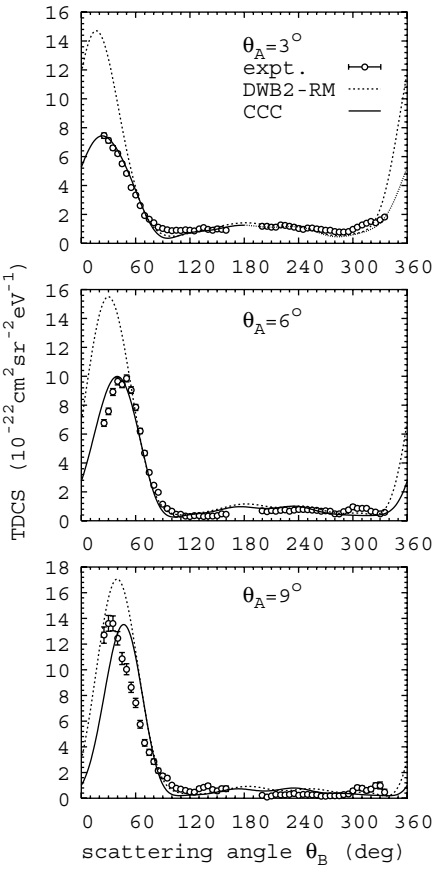

FIG. 1. Coplanar triply differential cross sections (TDCS) for 729.6 eV e-He ionization with E_A=500 eV and E_B=205 eV outgoing electrons. The relative measurements and the DWB2-RM calculation are due to Catoire *et al.* [10]. The CCC calculation is described in the text and was used to normalize the experiment at the binary maxima.

tion cross section, which is simply the sum of integrated cross sections of the positive-energy pseudostates. The CCC calculation yields 1.63×10^{-17} cm^2, which agrees well with the $1.68\pm0.08\times10^{-17}$ cm^2 measurement of Montague *et al.* [15].

The CCC-calculated TDCS are presented in Fig. 1. Since the measurements are relative and are not internormalized, we have normalized them to the CCC theory separately for each θ_A case by matching the binary maxima. Overall, we see quite a good shape agreement between CCC and experiment, particularly for the θ_A=3° and θ_A=6° cases. For θ_A=9° there is a visible angular shift in the position of the binary maximum. In going from θ_A=3° to θ_A=9° the two theories have the binary maxima shift systematically to higher angles, but not so in the experiment. At θ_A=6° theories predict this maximum at around 10° less than in experiment, yet for θ_A=9° the theories predict the maximum to be at around 20° more than in experiment. Another systematic discrepancy with experiment occurs around 100° where the theories consistently predict a lower minimum than what is found in the experiment. Additionally, the structure around 300° seen in the measurements is not able to be reproduced by theory.

Turning to the comparison between the two theories, we find the curious situation where agreement appears best away from the maxima. In the region of 60° to 300° the two theories are in remarkably good agreement. Given the relative nature of the experiment we can only use the experiment to decide which calculation yields better shape agreement with the measurements. For the θ_A=3° and θ_A=6° cases CCC yields slightly better shape agreement. For θ_A=9° both theories show a systematic difference with the measurements around the maximum of the cross section. Since the experimentally observed peak has moved substantially toward the smaller angles, this position is now closer to the prediction of the second-order distorted-wave Born approximation R-matrix (DWB2-RM) theory.

In conclusion, while the CCC method has generally improved the agreement with the experiment, and has provided what we believe to be accurate absolute values, there are still some unexplained discrepancies with the experiment. Given the systematic reduction in the quality of the shape agreement with increasing θ_A it would be interesting to have data for $\theta_A>9°$. Additionally, the presented CCC calculation is able to yield data for other values of E_B. Given the close-coupling nature of the CCC formalism agreement with experiment for one value of E_B is often indicative of a similar agreement for other values. Further such measurements and new calculations would be very helpful.

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