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LETTER TO THE EDITOR

Coplanar equal energy-sharing 64.6 eV e-He triple differential cross sections

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Abstract. Electron impact ionization of the ground state of helium is measured and calculated for the case of 64.6 eV incident electrons with coplanar outgoing 20 eV electrons. Various geometries are considered: symmetric, fixed θ_A and fixed $\theta_B - \theta_A$. The method of calculation is the convergent close-coupling theory. This theory is able to reproduce the angular profiles in essentially all of these geometries, yet it yields a constant factor of approximately two lower cross sections than experiment.

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Thus far the joint experimental and theoretical study of low to intermediate energy electron-impact ionization of helium has concentrated on the asymmetric energy-sharing kinematical regions (Röder *et al* 1996*a*, Röder *et al* 1996*b*). In these cases the convergent close-coupling (CCC) method yielded good agreement with experiment. However, it was noted that the agreement deteriorated when the total energy is shared more equally by the outgoing electrons.

Application of the CCC method at 100 eV (Bray and Fursa 1996*b*) and above (Bray and Fursa 1996*a*) did not show such problems. In fact we are confident that at these energies the CCC theory is able to yield accurate results irrespective of the scattering process of interest. However, there is a long way to go before we can be sure that the CCC theory will also work as well at lower energies. A detailed study of the double differential cross sections (DDCS) at the energy range from threshold to 100 eV has shown that the CCC theory, while yielding correct angular distributions, predicts cross sections that are too low in the equal energy-sharing kinematical region (Röder *et al* 1997). This conclusion is consistent with the earlier findings (Röder *et al* 1996*a*). The purpose of this letter is to present accurate and extensive triple differential cross section (TDCS) measurements at the intermediate energy of 64.6 eV for the equal energy-sharing kinematical region, together with the CCC calculations, thus enabling the most stringent test to date of the CCC theory of ionization.

The details of the CCC theory for electron impact ionization have been given by Bray and Fursa (1996*a*). This earlier work builds on the implementation of the CCC method for electron-impact excitation of hydrogen (Bray and Stelbovics 1992) and helium (Fursa and Bray 1995). The idea is similar to that of Curran and Walters (1987). The total wave function is expanded in a set of N pseudostates ϕ^N_{nls}, with associated energies ϵ^N_{nls}, obtained by diagonalizing the target Hamiltonian in a square-integrable basis. However, our approach does not involve reconstruction of this wave function. We rely on the close-coupling formalism to yield accurate T-matrix elements at the target-space energies ϵ^N_{nls}, and use them directly to define the (e,2e) scattering amplitudes

$$f^N_s(\mathrm{k},\mathrm{q}) \approx \sum_{l=0}^{l_{\max}} \langle \mathrm{q}_s|\phi^N_{n_q ls}\rangle \langle \mathrm{k}\phi^N_{n_q ls}|T|\phi^N_{n_i l_i s_i}\mathrm{k}_i\rangle. \qquad (1)$$

Here the projectile-space electron is denoted by a plane wave $|\mathrm{k}\rangle$, and the target-space continuum wave $|\mathbf{q}_s\rangle$ is a frozen-core two-electron continuum wave (Bray and Fursa 1996*a*). Note that in practice we solve the close-coupling equations in the distorted-wave formalism. This is done purely for numerical reasons and our results are independent of whether $|\mathrm{k}\rangle$ is a plane or a distorted wave.

In the case of atomic hydrogen $|\mathbf{q}_s\rangle$ would be just a pure Coulomb wave with $s = 1/2$. For helium the spins $s = 0, 1$ are involved. The T-matrix is obtained for a given total spin ($S = 1/2$ in the present case), thus the scattering amplitude $f^N_s(\mathrm{k},\mathrm{q})$ is a coherent

sum of the direct and exchange amplitudes. For each s and $l = 0, \ldots, l_{\max}$, where $l_{\max}$ is the maximum target-space orbital angular momentum used in the coupled equations, the continuum-wave energy $\epsilon_q = \epsilon^N_{n_q ls}$. The approximation in (1) is due to the fact that if $\epsilon^N_{n_q ls} = \epsilon_q$, then the overlap $\langle \mathbf{q}_s | \phi^N_{nls} \rangle$ is negligible for all $n \neq n_q$. In order to ensure that $\epsilon^N_{n_q ls} = \epsilon_q$ for each l, s some interpolation is necessary (Bray and Fursa 1996*a*).

We use the CCC e-2e ionization amplitude (1) to define the TDCS. In atomic units the TDCS is given by

$$\frac{d^3\sigma^N_{\rm CCC}(\mathbf{k},\mathbf{q})}{d\Omega_k d\Omega_q de_q} = (2\pi)^4 \frac{kq}{k_i} \sum_s |f^N_s(\mathbf{k},\mathbf{q})|^2. \tag{2}$$

An important, but surprising, feature of our approach is that we have a clear distinction between the primary (scattered) and the ejected (target) electrons. This is due to the unitarity of the close-coupling formalism and has been discussed in detail elsewhere (Bray and Fursa 1995, Bray and Fursa 1996*a*). For a given total energy $E = \epsilon_q + k^2/2$ the CCC theory gives rise to two processes originating from different T-matrix elements corresponding to target-space energies ϵ^N_{nls} and $E - \epsilon^N_{nls}$. The first process is described by the amplitude $f^N_s(\mathbf{k},\mathbf{q})$ and has the primary electron with momentum $\mathbf{k}$ and the ejected electron with momentum $\mathbf{q}$. The second process is described by the amplitude $f^N_s(\mathbf{q},\mathbf{k})$ and has the primary electron with momentum $\mathbf{q}$ and the ejected electron with momentum $\mathbf{k}$. These two theoretically distinct processes cannot be distinguished experimentally due to the indistinguishability of the detected electrons. Therefore, when comparing theory with experiment, we form an incoherent sum of the cross sections for the two theoretically distinct processes

$$\frac{d^3\sigma^N(\mathbf{k},\mathbf{q})}{d\Omega_k d\Omega_q de_q} = \frac{d^3\sigma^N_{\rm CCC}(\mathbf{k},\mathbf{q})}{d\Omega_k d\Omega_q de_q} + \frac{d^3\sigma^N_{\rm CCC}(\mathbf{q},\mathbf{k})}{d\Omega_k d\Omega_q de_q}. \tag{3}$$

Note that this has to be done regardless of whether exchange between the projectile and target electrons has, or has not, been included in the close-coupling calculation. In the case of equal-energy outgoing electrons $q = k$. For the symmetric geometry (see figure 4) the two CCC terms in (3) are the same. However, for other geometries these terms are substantially different due to the interchange of $\hat{\mathbf{k}}$ and $\hat{\mathbf{q}}$. Convergence in (3) is tested by simply increasing the basis size N.

The experimental apparatus has been described in some detail by Röder *et al* (1996*b*). Rösel *et al* (1992) and Ehrhardt *et al* (1986). Here we shall just concentrate on the method of normalization.

The TDCS are related to the count rate of true coincidences $N_{\rm TDCS}$ by

$$N_{\rm TDCS} = \frac{d^3\sigma}{d\Omega_A d\Omega_B de} \times (n\ N_e\ l) \times (\Delta\Omega\,\varepsilon)_A \times (\Delta\Omega\,\varepsilon)_B \times \Delta E_{\rm TDCS}, \tag{4}$$

where n is the gas density in the interaction region, N_e is the rate of primary electrons, l is the effective overlap length of the gas and electron beams, $(\Delta\Omega\,\varepsilon)_{A,B}$ is the product

of the solid angle of detection and the detection efficiency of the analysers and $\Delta E_{\rm TDCS}$ is the energy resolution. The product $(n\ N_e\ l)$ is determined by measuring the current of the ions produced by electron impact at the incident energy of interest (E_0) and dividing the ion rate $N_{\rm ion}$ by the accurately determined total ionization cross section $\sigma_{\rm tot}$ of Shah *et al* (1988)

$$N_{\rm ion} = \sigma_{\rm tot} \times (n\ N_e\ l). \tag{5}$$

The energy resolution $\Delta E_{\rm TDCS}$ is essentially determined by the width of the elastic peak and the energy binding spectrum (Rösel *et al* 1992). The term $(\Delta\Omega\,\varepsilon)_{A,B}$ depends only on the analyser properties, and may be determined by the use of known absolute DDCS at high incident energies with same (20 eV in our case) secondary energies (Röder *et al* 1997). This is done separately for each detector A and B. We then have all of the parameters necessary to determine an absolute measured TDCS via (4). The estimated error in such a procedure is typically of order 25%-30%.

In figure 1 we give the excited-state energies, relative to the He^+ core, arising in the 113-state (CCC(113)) and the 101-state (CCC(101)) calculations. The difference between the two is that the former has more S-, P-, D-, F- and G-states than the latter, but has no H-states. The exponential fall-off in the Laguerre basis (Fursa and Bray 1995) has been varied slightly so as to ensure that for each target symmetry one of the levels was near 20 eV ($E/2$). This way the dependence of the results on the interpolation method (Bray and Fursa 1996*a*) is minimised.

The measurements were performed in three different coplanar geometries. In one the angular separation between the two detectors was kept constant (fixed $\theta_B - \theta_A$), with the two detectors rotated together in the plane. Another had a fixed angle θ_A for one detector, with the other rotated in the plane. The last is the so-called coplanar symmetric geometry, where both detectors are rotated in the plane on either side of the incident electron beam with $\theta_A = -\theta_B$.

The measurements and calculations for the former geometry are given in figure 2. Excellent shape agreement is found between the theory and experiment. However, the results of the barely distinguishable CCC calculations are a constant factor of approximately two lower than the measurements. The convergence of the CCC(113) and CCC(101) calculations is particularly noteworthy. Even though we are dealing with 20 eV outgoing electrons, using target-space angular momentum $l \leq l_{\max} = 4$ is clearly sufficient. We believe this to be due to unitarity of the CCC formalism. Since the target- and projectile-spaces are distinguishable unitarity ensures that little flux is lost from the initial $l = 0$ target ground state to higher l-states. The projectile-space electron was treated with 31 partial waves.

For the $\theta_B - \theta_A = 90°$ case, in addition to the summed CCC results given according to (3), we give the two "raw" CCC components, labeled raw(113). We see that the

sum of these two terms is crucial in order to achieve agreement with the experimental profile. For contrast, in the $\theta_B - \theta_A = 120°$ case, we combine the amplitudes $f_s^N(\mathbf{k},\mathbf{q})$ and $f_s^N(\mathbf{q},\mathbf{k})$ coherently, with the result labeled by coh(113). Clearly, this yields an incorrect profile.

The results for the fixed θ_A geometry are given in figure 3. Once again we find good shape agreement between the measurements and the two CCC calculations. The factor by which the magnitudes differ is the same. This must be the case for all three geometries considered since they have overlapping points. At $\theta_A = 30°$ there appears to be a discrepancy in the predicted ratio of binary ($\theta_B = -60°$) and recoil ($\theta_B = 150°$) peaks. However, if we set $\theta_A = 30°$ in the $\theta_B - \theta_A = 90°$ and 120° cases of figure 2 then we obtain substantially better agreement with experiment in the recoil peak angular range. The reason for this inconsistency in the measurements is likely to be due to an imperfect symmetric adjustment of the spectrometer during the measurement of the fixed $\theta_A = 30°$ case. As discussed by Röder *et al* (1996*b*) the quality of this kind of measurement depends strongly on the symmetry of the DDCS countrate on both sides of the primary beam. The DDCS varies very rapidly around $\theta_A = \pm 30°$. A small deviation could easily lead to a drop in the recoil- and an increase in the binary-region of the cross section, or vice versa.

The bumps around $\theta_B = 0°$ in the calculations of the $\theta_A = 30°$ case are unphysical and show that this angular region is particularly sensitive to the size of the calculation. At $\theta_B = \theta_A$ the cross section should be identically zero as it corresponds to same-energy electrons emerging in the same direction. This is clearly not the case at $\theta_A = 30°$ but improves with larger θ_A.

This sensitivity to small θ_A is even more evident in the coplanar symmetric geometry, presented in figure 4. We see that the two calculations produce very different results at $\theta_A = 0°$. Both should yield identically zero here. The best of the calculations is the CCC(113), indicating that long-range electron-electron correlation is best taken into account with large basis sizes within a target symmetry. This ensures best square-integrable representation of the true continuum wave. For this geometry we are also able to compare with the data of Murray and Read (1993), normalised using the 100 eV absolute data of Gélébart and Tweed (1990). It also yields excellent agreement in profile with the present measurements and calculations, but is a factor of two or so higher than the present measurements.

Faced with discrepancy in the absolute values from different experimental groups and such remarkable shape agreement with the CCC theory, it is tempting to suggest that the correct magnitude is given by the theory. Particularly so since we know that the CCC theory yields correct total ionization cross sections (Fursa and Bray 1995). However, we do not believe this to be the case. A detailed study of double and single differential cross sections (Röder *et al* 1997) has shown that the CCC theory consistently

predicts magnitudes that are too low in the near equal energy-sharing kinematical region, while yielding correct magnitudes in the case of asymmetric energy-sharing. Why this should be the case is currently under intense investigation. We believe that it relates to fundamental aspects of calculation of ionization via the close-coupling formalism. Nevertheless, we find the quality of the shape-agreement over the entire (θ_A, θ_B) plane to be quite remarkable. It will be interesting to apply the same calculations to the out-of-plane measurements of Murray and Read (1993).

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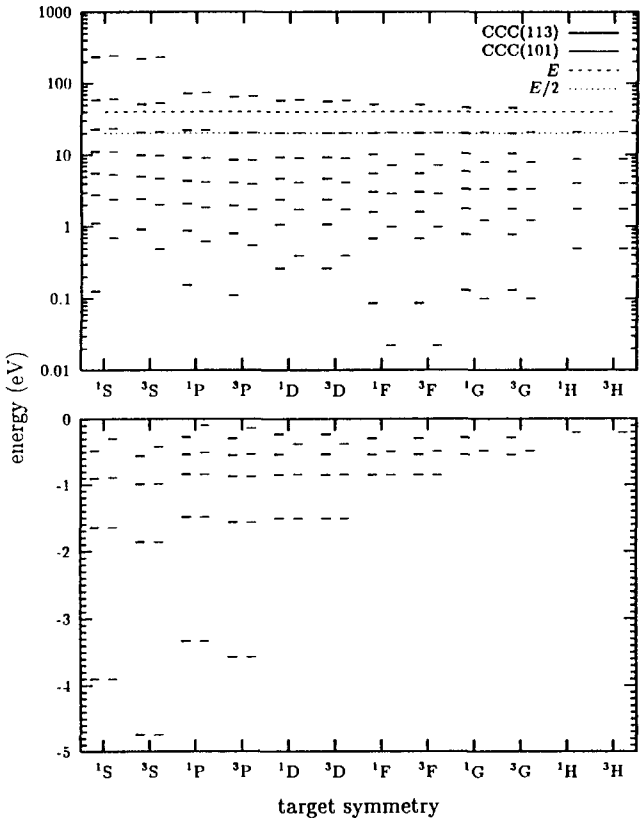

Figure 1. Excited-state energy levels arising in the CCC(113) and CCC(101) calculations. For 64.6 eV electron-impact ionization of the helium ground state the total energy E is 40 eV.

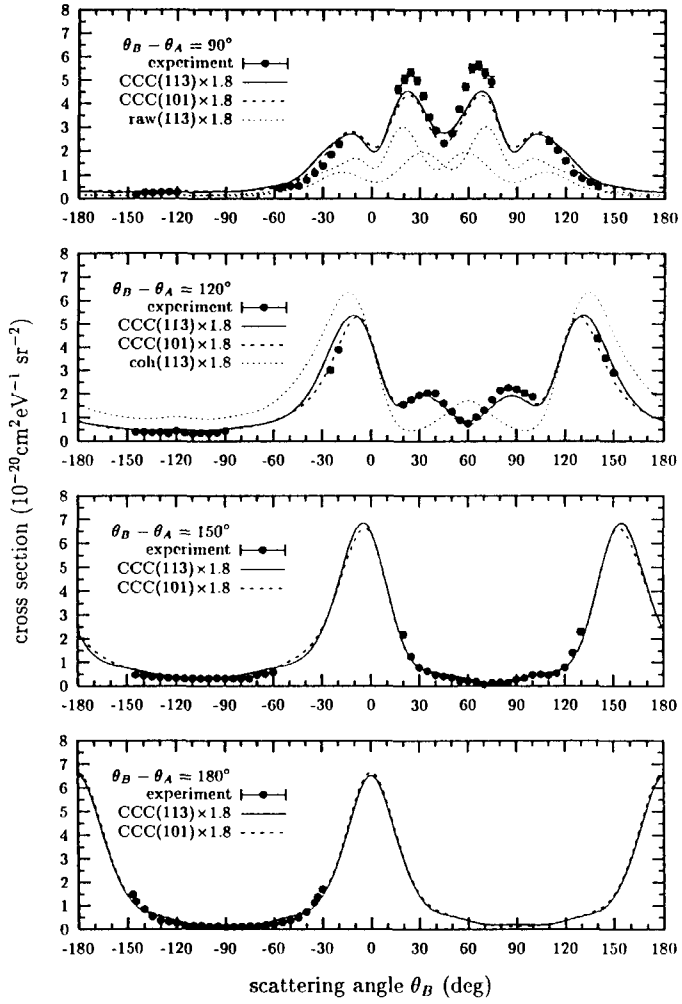

Figure 2. Coplanar triple differential cross sections at specified fixed values of $\theta_B - \theta_A$ for electron-impact ionization of helium at 64.6 eV with 20 eV outgoing electrons. See text for details of experiment and calculations.

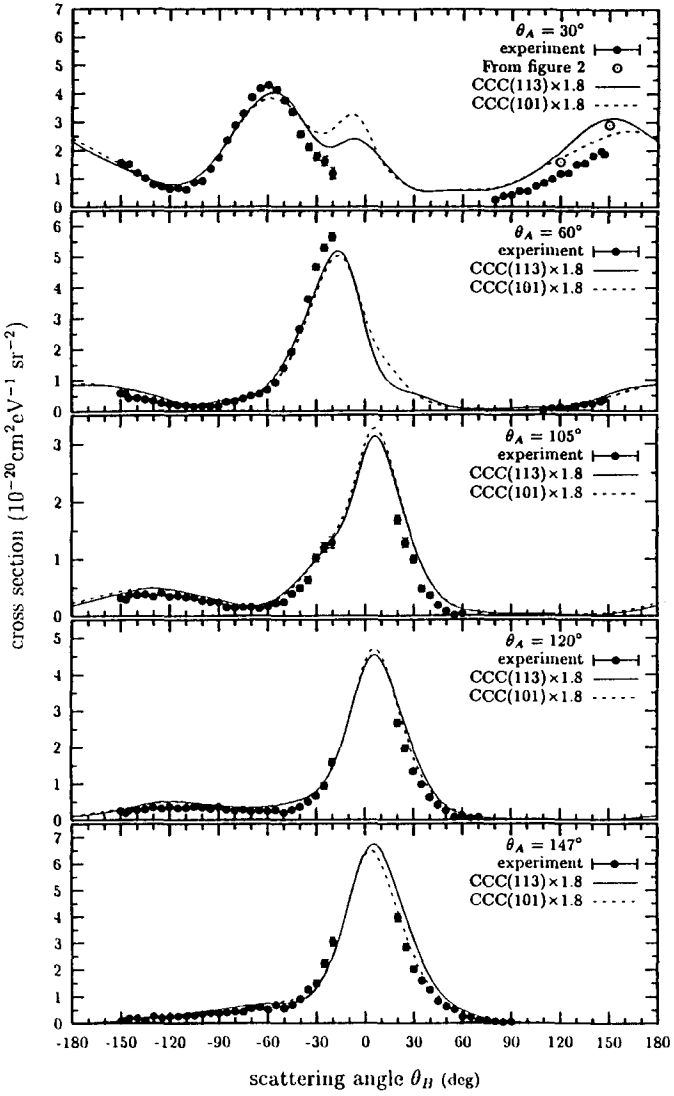

Figure 3. Coplanar triple differential cross sections at specified fixed values of θ_A for electron-impact ionization of helium at 64.6 eV with 20 eV outgoing electrons. See text for details of experiment and calculations.

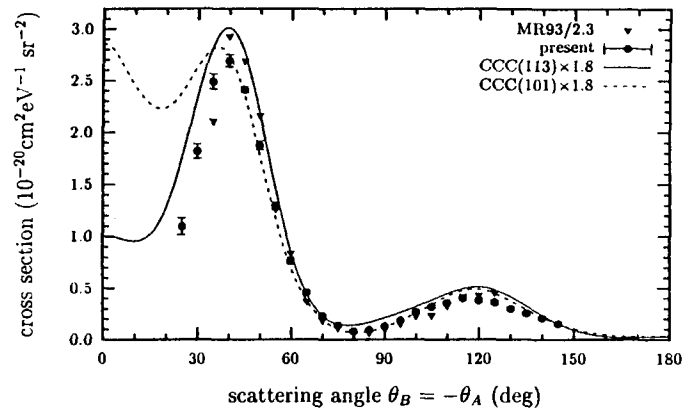

Figure 4. Coplanar symmetric triple differential cross section for electron-impact ionization of helium at 64.6 eV with 20 eV outgoing electrons. See text for details of present experiment and calculations. The data labeled MR93 is due to Murray and Read (1993).