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J. Roder
Fachbereich Physik, Universitat Kaiserslautern, Germany

H. Erhardt
Fachbereich Physik, Universitat Kaiserslautern, Germany

Cheng Pan
University of Nebraska - Lincoln

Anthony F. Starace
University of Nebraska-Lincoln, astarace1@unl.edu

Igor Bray
Flinders University of South Australia, i.bray@curtin.edu.au

See next page for additional authors

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Authors

J. Roder, H. Erhardt, Cheng Pan, Anthony F. Starace, Igor Bray, and Dmitry V. Fursa

Absolute Triply Differential (*e*,2*e*) Cross Section Measurements for H with Comparison to Theory

J. Röder,[1] H. Ehrhardt,[1] Cheng Pan,[2,*] Anthony F. Starace,[2] Igor Bray,[3] and Dmitry V. Fursa[3]
[1]*Fachbereich Physik, Universität Kaiserslautern, D-67663 Kaiserslautern, Germany*
[2]*Department of Physics and Astronomy, The University of Nebraska, Lincoln, Nebraska 68588-0111*
[3]*Electronic Structure of Materials Centre, The Flinders University of South Australia, G.P.O. Box 2100, Adelaide 5001, Australia*

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Absolute triply differential $(e,2e)$ cross section measurements are presented for H (for incident energies, E_0, of 15.6 and 17.6 eV) for equal energy sharing and the $\theta_{12} = \pi$ configuration. Results of distorted partial wave calculations agree with the measurements; those of convergent close coupling calculations agree with the relative angular distributions, but are lower than experiment by factors of from 2 to 7. Relative experimental results for H for $E_0 = 14.6$ eV show a qualitative change in shape, which agrees with theory. Implications of the absolute experimental results for the range of validity of the Wannier threshold law are discussed. [S0031-9007(97)03959-8]

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The electron impact ionization, or $(e,2e)$, process in H, like the photo-double ionization process in He, is one of the most fundamental ways of investigating three-body Coulomb dynamics, particularly for relatively low incident energies. Interest in triply differential $(e,2e)$ measurements in both H and He was sparked in the late 1980's by measurements taken at only 4 eV above the ionization thresholds [1,2]. These showed that the shapes of the angular distributions depend on the target even though the asymptotic Coulomb fields experienced by the three final state particles are target independent. While theoretical calculations [3–6] were able to replicate reasonably well the experimentally observed $(e,2e)$ angular distributions, the first absolute measurements, for He [7,8], agreed with only two of these [4,6]. The implicit implication was that accurate accounting of target effects on the various electronic partial waves as well as treatment of electron-electron interactions are necessary to obtain agreement with absolute data and that omission of these effects can lead to disagreement with experiment by factors of 2–200 [9]. In response to these first absolute measurements for He, theorists have since devoted increased attention to providing not only accurate angular distributions but also accurate absolute cross sections [8,10–12]. Absolute measurements near threshold are also necessary to determine the threshold law for fragmentation of three-body Coulomb systems. According to the Wannier-Peterkop-Rau (WPR) theory [13–15] for the threshold law, the triply differential cross sections for $(e,2e)$ processes should vary with energy as $E_{\rm ex}^{-0.373}$ [1,14(b)], where $E_{\rm ex}$ is the energy "excess" above threshold. The absolute measurements for He, however, are not yet sufficiently close to threshold to verify this predicted energy dependence [16].

We report here the first absolute measurements for the triply differential cross section (TDCS) for the $(e,2e)$ process in H at excess energies of 2 and 4 eV. In addition, new relative measurements for the TDCS in H are presented for incident energies of 14.6, 20, and 25 eV, the first of which confirms earlier predictions of a qualitative change in shape very close to threshold [4(b)]. In all of the measurements presented, the two final state electrons share the excess energy equally and depart in opposite directions (i.e., $\theta_{12} = \pi$). The new measurements are compared here with results of two theoretical approaches: the distorted partial wave (DPW) approach of Pan and Starace [4] and the convergent close coupling (CCC) approach of Bray *et al.* [17]. At low energies, the DPW approach [4] has provided an interpretation of the observed differences in the $(e,2e)$ TDCS's for H and He [2] in terms of partial wave phase shifts; its predictions have also been found to be in excellent agreement with the first absolute TDCS results for He [7,8]. At high energies, the CCC approach [17,18] provides accurate results in excellent agreement with all experimental features.

The details of the determination of accurate absolute TDCS's have been given by Rösel *et al.* [19]. Absolute values are obtained with the assistance of accurate reference data on total ionization cross sections $\sigma_{\rm ion}$, rather than attempting to measure all aspects of the scattering process. As in the case of rare gases, the dependence of the absolute values on the product of the target density $n_{\rm H}$, the scattering length ℓ, and the rate of primary electrons N_e may be inferred by measuring the ion count rate $N_{\rm ion}$ via

$$N_{\rm ion} = n_{\rm H} N_e \ell \sigma_{\rm ion} . \qquad (1)$$

In the case of atomic hydrogen there is a further complication due to the existence of molecular hydrogen in the beam. This doesn't affect the measurement of the angular dependencies, since the 1.8 eV difference in the ionization potentials of atomic and molecular hydrogen is much larger than the 300 meV energy resolution of the electron spectrometers. However, absolute normalization is affected due to the measured ion current arising from both the H^+ and H^{2+} ions. This requires a correction, which may be determined by measuring the disassociation rate α [$= H/(H + H_2)$] in the scattering center. In this case

$$\sigma_{\mathrm{ion}} = \sigma_{\mathrm{ion}}^{H} + \sigma_{\mathrm{ion}}^{H_2}(1 - \alpha)/\alpha . \tag{2}$$

Accurate values of the total electron-impact ionization cross sections $\sigma_{\mathrm{ion}}^{H}$ and $\sigma_{\mathrm{ion}}^{H_2}$ have been tabulated in the literature over an extensive energy range. The disassociation rate was measured with an ion spectrometer of the type described by Köllmann and Grüter [20], which has been widely used in atom-atom and atom-ion beam experiments, and was found to be $\alpha = (18.5 \pm 1.85)\%$. All other parameters that affect the absolute cross sections are independent of the target and can be determined, as in Ref. [19], by measuring cross sections for helium using exactly the same adjustments as for the target of interest. This means, for example, that the absolute normalization of the TDCS of atomic hydrogen at $E_0 = 17.6$ eV in equal energy sharing conditions uses nearly all of the measurements required for the absolute determination of the TDCS of helium at 28.6 eV, also in the equal energy sharing conditions. In both cases the analyzers detect electrons of 2 eV. Parallel to the measurements for the absolute TDCS of atomic hydrogen at 15.6 and 17.6 eV, we have measured [21] the absolute TDCS of helium at corresponding energies (only the ion rate and the coincidence rate had to be measured additionally). The TDCS's of helium at 26.6 and 28.6 eV, in the equal energy sharing conditions, determined in this work as a check of consistency, are in agreement with the results obtained earlier by Rösel *et al.* [22].

The theoretical approaches whose results are compared to the experimental measurements reported here have been described in detail elsewhere. Thus we merely summarize briefly their main features. In the DPW approach, the incident electron is expanded in LS-coupled partial waves in which each radial wave function is calculated in the Hartree-Fock (HF) potential V_{HF} describing the interaction of the incident electron with the target electron. The final-state wave function Ψ_f^- is also an expansion in independent-electron states for each of the two continuum electrons, in which their orbital and spin angular momenta are coupled to partial waves characterized by L and S, which are the total orbital and spin angular momenta of the system. The major approximation to Ψ_f^- is the replacement of the exact Coulomb interaction between the two continuum electrons by a variationally determined screening potential [23–25]. The DPW approach thus treats distortion, nonlocal exchange interactions, both singlet and triplet partial waves, and mutual screening interactions using effective charges which satisfy proper asymptotic boundary conditions. Further details are presented in [4,26].

In the CCC approach (see [18] for details) the total wave function is expanded in a set of square-integrable (L^2) states, with the resultant coupled equations for the T matrix solved in momentum space. The ionization amplitudes are constructed directly from the amplitudes corresponding to the excitation of the positive-energy pseudostates. The number of states N is increased until the CCC(N) results converge to a desired accuracy. The usage of the L^2 expansion leads to the final channels being a product of an asymptotically plane wave for one (projectile-space) electron and, in the case of hydrogen, a Coulomb wave for the other (target-space). The CCC results are independent of whether the projectile-space electron is represented by a distorted or a plane wave. One may expect that such an asymmetric treatment of the outgoing electrons would yield poor angular distributions in the case of equal-energy-sharing kinematics. However, the CCC theory has already obtained excellent agreement with the experimental profiles for all coplanar geometries in the case of 64.6 eV e-He ionization with 20 eV outgoing electrons, though a factor of 2 less in magnitude [27]. Here we concern ourselves with just the coplanar $\theta_{12} = \pi$ geometry.

Figure 1 shows equal energy-sharing e-H TDCS [28] measurements as well as both DPW and CCC results for incident energies of 14.6, 15.6, 17.6, 20, and 25 eV and for $\theta_{12} = \pi$. The measurements at 15.6 and 17.6 eV are absolute with error estimates shown. The relative measurements at the other energies are normalized to the DPW results at $\theta_1 = 90°$. The statistical errors in the relative measurements are of similar magnitude to the size of the symbols denoting the experimental values. In general, for all energies both theoretical results describe accurately the measured angular distribution. However, at all energies the CCC results must be multiplied by factors of 2–7 to agree in magnitude with either the absolute measurements or with the DPW results. The error bars on the absolute measurements are sizable: $\pm 35\%$ at $E_0 = 15.6$ eV and $\pm 40\%$ at $E_0 = 17.6$ eV. At 17.6 eV, the DPW results fall within the error bars at all angles. At 15.6 eV, the DPW results are presented multiplied by a factor of 2 and so are somewhat below the experimental points. The relative measurements at 14.6 eV indicate that the shape of the angular distribution undergoes a qualitative change: the bowl shape at $\theta_1 = 90°$ flattens out. This partially confirms DPW predictions made for 14.1 eV in Ref. [4(b)] that at lower energies the angular distribution at $\theta_1 = 90°$ has a small local maximum, as in the case of He. As shown in Fig. 1, at 14.6 eV the DPW results predict a flat-bottomed curve while the CCC results already predict a small local maximum.

As mentioned above, the TDCS for $(e, 2e)$ processes for the $\theta_{12} = \pi$ geometry has an energy dependence of $E_{\mathrm{ex}}^{-0.373}$ as $E_{\mathrm{ex}} \to 0$ in the WPR theory owing to the predicted rapid narrowing of the width of the distribution with respect to θ_{12} in the region of $\theta_{12} = \pi$. The DPW results, however, which employ an effective screening approximation [23–25], are independent of E_{ex} as $E_{\mathrm{ex}} \to 0$. In Fig. 2 we present the energy dependence of the $(e, 2e)$ TDCS's for H in the near threshold energy region for two geometries: $\theta_1 = 90°$ and $\theta_1 = 30°$ with $\theta_{12} = \pi$.

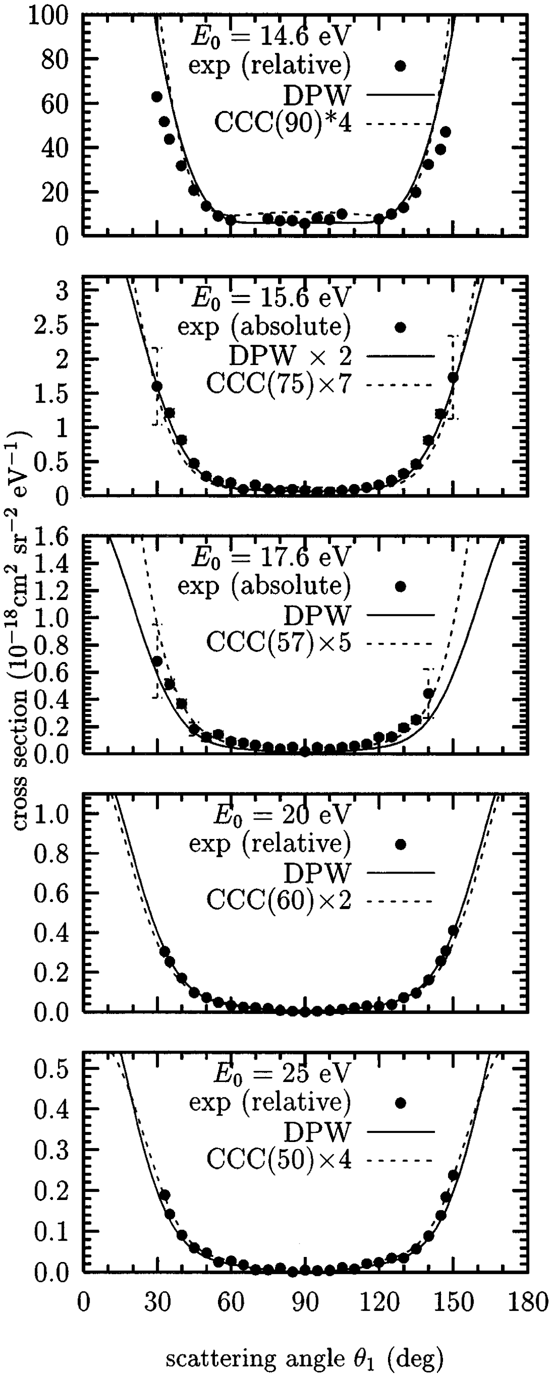

FIG. 1. Equal energy sharing e-H triply differential cross sections at the indicated projectile energies. See text for detail of theory and experiment.

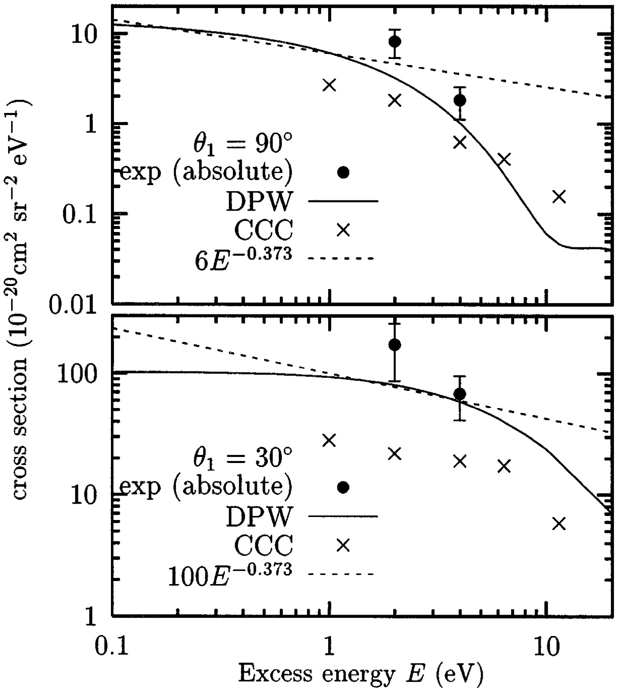

FIG. 2. Equal energy sharing e-H triply differential cross sections at $\theta_1 = 90°$ and 30° in the Wannier ($\theta_{12} = \pi$) geometry as a function of excess (total) energy.

The $\theta_1 = 90°$ figure documents the finding shown for an incident energy of 14.6 eV in Fig. 1 that the TDCS is developing a local maximum at $\theta_1 = 90°$, as shown by the rising DPW and CCC predictions as $E_{\mathrm{ex}} \to 0$. Owing to this dynamical change in the TDCS it is difficult to use the $\theta_1 = 90°$ figure to make any statement on the WPR threshold law. In contrast, the $\theta_1 = 30°$ figure shows the expected leveling off of the DPW predictions as $E_{\mathrm{ex}} \to 0$. In the latter figure the DPW results almost pass through the error bars of both of the present absolute measurements. The CCC results have the same energy behavior as the DPW results, but are lower in magnitude. As there are no theoretical predictions for the absolute value of the TDCS for $(e, 2e)$ processes in H that are consistent with WPR, we are only able to show with the dotted line the WPR prediction of -0.373 for the slope of the TDCS as $E_{\mathrm{ex}} \to 0$. For $\theta_1 = 30°$ this slope is consistent with both theoretical predictions as well as with the measured points in the energy region of 2 to 4 eV above threshold. Clear differences occur only for excess energies below 1 eV. In contrast, for $\theta_1 = 90°$ both theoretical predictions and the measured points are rising as $E_{\mathrm{ex}} \to 0$ faster than the WPR prediction in the region of the measurements. However, as discussed, this is a dynamical effect whose origin is outside WPR theory.

In summary, we report the first absolute measurements of the TDCS for $(e, 2e)$ processes for equal energy sharing and the $\theta_{12} = \pi$ geometry in H. As was the case for the first absolute measurements for such processes in He [7,8], these new results indicate that it is easier theoretically to predict accurate $(e, 2e)$ angular distributions than absolute cross sections. In particular, one of the leading theories for e-H and e-He scattering processes, the CCC theory, is shown to provide accurate angular distributions but incorrect absolute TDCS results (i.e., lower by factors of 2–7) in the energy region from threshold to 25 eV above. This is particularly remarkable given that the CCC theory predicts correct absolute total ionization cross sections

[10]. In contrast, the simpler DPW approach, which we have restricted to the $\theta_{12} = \pi$ geometry owing to the screening approximation it employs, gives reasonably accurate predictions of both the angular distribution and the absolute TDCS's over the entire energy region considered here. This success underlines the importance of treating distortion and nonlocal exchange effects in each partial wave for the $(e, 2e)$ process in addition to mutual screening effects. The present results indicate also that absolute measurements below 2 eV above threshold are necessary if the predictions of the WPR threshold law for $(e, 2e)$ TDCS's in H are to be confirmed. This is consistent with similar findings for He [16].

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*Present address: Joint Center for Radiation Therapy, Harvard Medical School, 330 Brookline Avenue, Boston, MA 02215.

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[28] The TDCS is differential in the momenta $\vec{k}_1$ and $\vec{k}_2$ of the two continuum electrons in the final state. All our results focus on the geometry $\hat{k}_1 = -\hat{k}_2$, in which the electrons depart in opposite directions. Thus $\hat{k}_1 \cdot \hat{k}_2 \equiv \cos\theta_{12} = -1$, from which arises the terminology "$\theta_{12} = \pi$ geometry." With respect to the incident electron direction (taken as the z axis), one may define $\hat{k}_1 \equiv (\theta_1, \varphi_1)$ and $\hat{k}_2 \equiv (\theta_2, \varphi_2)$ in the usual way. In the $\theta_{12} = \pi$ geometry, $\theta_1 + \theta_2 = 180°$ and $\varphi_2 = \varphi_1 + 180°$.