Triply Differential Cross Sections for the Ionization of Helium by Fast Electrons

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The triply differential cross section for the single ionization of helium by 500-eV electrons has been measured in a coplanar asymmetric geometry and analyzed by using a second Born-approximation treatment. It is found that these theoretical predictions concerning the angular positions, shapes, and magnitudes of both the binary and recoil peaks are in good agreement with experiment.

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The goal of the present Letter is to improve our understanding of electron-impact ionization, a process which has posed considerable challenge to theory in recent years. We present new experimental and theoretical results concerning the triply differential cross section for a fundamental ionization process, namely the single ionization of helium by electron impact leaving the He^+ ion in the ground state,

$$e^- + \mathrm{He}(1^1S) \rightarrow \mathrm{He}^+(1s) + 2e^-.$$

The triply differential cross section is the most sensitive test for a theoretical treatment of the electron-impact ionization,[1] since in a coincidence experiment all kinematic parameters are determined, namely the energy E_0 of the incident electron and the energies E_A and E_B and angles θ_A and θ_B of the two outgoing electrons. The corresponding momenta are $\vec{k}_0$, and $\vec{k}_A$, and $\vec{k}_B$. As a result of the energy resolution of E_A as well as E_B it is insured that the ion is in its ground state. For such an experiment with totally determined kinematics the scattering amplitude is tested without integrating with respect to energies and angles.

In the case of high energy (E_0 large), symmetric kinematics ($E_A = E_B$, $\theta_A = \theta_B = \theta$), and large momentum transfer ($\theta \geq 30°$), impulse-type approximations adequately describe the triply differential cross section. This fact has been used to analyze the momentum density distributions of the target electrons via $(e,2e)$ spectroscopy studies.[2]

Now, it is known from singly and doubly differential cross sections that for intermediate and high E_0 most ionization events occur in such a way that one of the outgoing electrons is fast (E_A) and is scattered into a narrow cone θ_A with respect to the incoming electron, whereas the other outgoing electron is slow (E_B) and is ejected into a large angle θ_B. Hence, the experimental setup for the measurement of the triply differential cross section has to ensure an extreme asymmetric geometry in order to detect the majority of ionization processes. In this Letter we shall focus our attention on such asymmetric coplanar events for which the magnitude of the momentum transfer $\vec{k}_{0A} = \vec{k}_0 - \vec{k}_A$ is small ($\lesssim 1$ a.u.).

The experimental system has been described in detail in previous publications.[1,3] In short, the electron gun is fixed in position and produces an electron beam of approximately 10^{-7} A with ca. 200-meV energy spread. This beam crosses an atomic beam (10^{-2} Torr) at right angle. The two outgoing electrons are registered individually by the detectors A and B, both containing 127° energy analyzers and capable of being rotated in the angular range from 0° to 150° with respect to the incident electron beam. The angular uncertainty of each detector is ca. 1°, and the time resolution of the coincidence unit 6 nsec. The gun and the two detectors operate in one plane. For the measurement of a triply differential cross section the parameters E_0, E_A, E_B, and θ_A are fixed and the detector B is swept with respect to the angle θ_B for the registration of the intensity of the slow electrons.

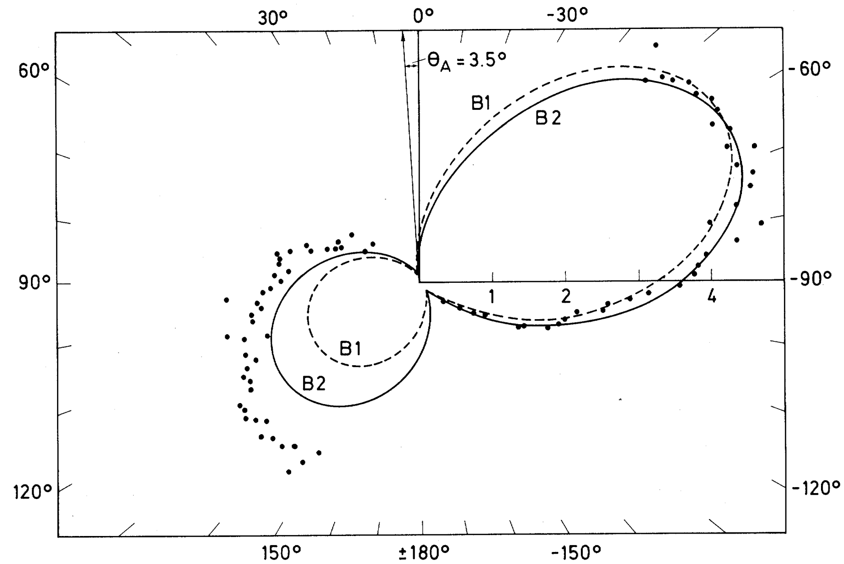

FIG. 1. The triply differential cross section $d^3\sigma/d\Omega_A d\Omega_B dE$ (in a.u.) for the ionization of helium by electron impact, for the case $E_0 = 500$ eV, $E_B = 5$ eV, and $\theta_A = 3.5°$. The dashed curve refers to the first Born approximation ($\times 0.87$); the solid curve, to the second Born approximation of Eq. (1), calculated with an average excitation energy $\bar{w} = 0.9$ a.u. The dots correspond to the experimental data. All results are normalized to the same value at $\theta_B = -60°$, near the maximum of the binary peak.

A typical result (dots) is shown in Fig. 1 in the form of a polar graph, for an incident energy of $E_0 = 500$ eV, an ejected electron energy of $E_B = 5$ eV and a scattering angle of $\theta_A = 3.5°$. The graph shows a strong angular correlation between the two outgoing electrons. The angular distribution of the ejected electrons exhibits a lobe in the right-hand half-plane, whose maximum is near the direction of $\vec{k}_{0A}$. This peak is called the binary peak, since it originates mainly from the electron-electron interaction during the collision. The so-called recoil peak is positioned in the left-hand half-plane. It is qualitatively explained by momentum transfer to the ion.

In the last decade, several attempts have been made to calculate[4] such triply differential cross sections for helium for incident energies $E_0 = 30$ to 250 eV and many parameter values of E_A, E_B, and θ_A. In general, the binary peak was described quite well, whereas severe discrepancies remained concerning the size, shape, and position of the recoil peak. The present measurements have been made preferentially to study the structure of the recoil peak as a function of $\vec{k}_{0A}$ and $\vec{k}_B$.

The theoretical calculations of this paper have been carried out by using the eikonal-Born series method.[5-6] According to this approach, the direct scattering amplitude is obtained by adding the first Born term, the second Born term, and the third-order term of the Glauber series. However, in the present coplanar asymmetric geometry, where θ_A is small and the energy E_B of the ejected electron is small compared to that of the scattered electron, the third Glauber term is small. Moreover, in this geometry exchange effects are also negligible. Finally, the use of the closure approximation in calculating the second Born term is expected to be best when the energy of the ejected electron is small, as in the present case. We have therefore obtained our theoretical triply differential cross sections by using the expression[7]

$$\frac{d^3\sigma}{d\Omega_A d\Omega_B dE} = \frac{k_A k_B}{k_0} |f_{B1} + f_{SB2}|^2, \tag{1}$$

where f_{B1} is the first Born approximation to the direct scattering amplitude,

$$f_{B1} = -(2\pi)^{-1} \left\langle \exp(i\vec{k}_A \cdot \vec{r}_0)\psi_f(\vec{r}_1, \vec{r}_2) \left| \frac{1}{r_{01}} + \frac{1}{r_{02}} \right| \exp(i\vec{k}_0 \cdot \vec{r}_0)\psi_i(\vec{r}_1, \vec{r}_2) \right\rangle, \tag{2}$$

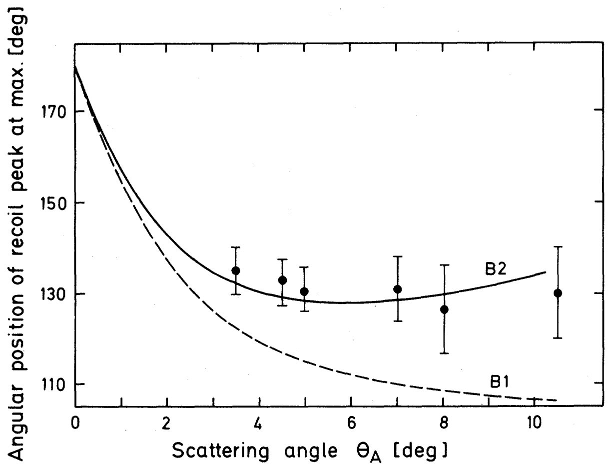

FIG. 2. The angular position of the maximum of the recoil peak as a function of the scattering angle θ_A, for the case $E_0=500$ eV and $E_B=10$ eV. The dashed curve refers to the first Born approximation (direction $-\vec{k}_{0A}$); the solid curve, to the second Born approximation of Eq. (1) with $\bar{w}=0.9$ a.u. The dots represent the measurements.

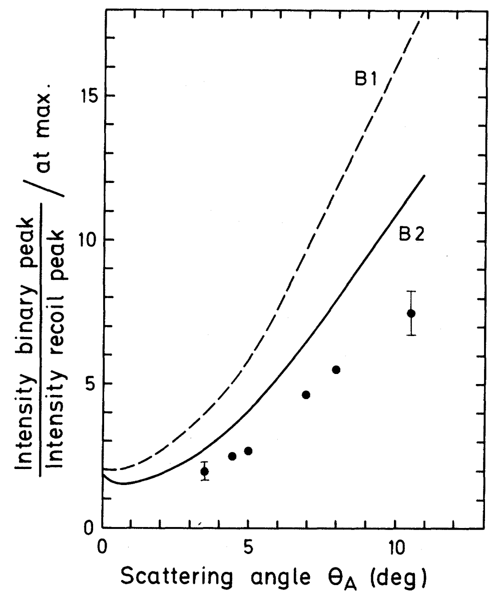

FIG. 3. The ratio of the intensity of the binary peak to that of the recoil peak, at the maximum, as a function of the scattering angle θ_A, for the case $E_0=500$ eV and $E_B=10$ eV. The experimental data (dots) are compared with the first Born approximation (dashed line) and the second Born approximation (solid line).

and f_{SB2} refers to the second Born term of the direct scattering amplitude, calculated in the closure approximation,

$$f_{SB2}=(8\pi^4)^{-1}\int d^3q\,\frac{1}{q^2-p^2-i\epsilon}\left\langle\psi_f(\vec{r}_1,\vec{r}_2)\right|\left\langle\exp(i\vec{k}_A\cdot\vec{r}_0)\left|\frac{1}{r_{01}}+\frac{1}{r_{02}}-\frac{2}{r_0}\right|\exp(i\vec{q}\cdot\vec{r}_0)\right\rangle$$
$$\times\left\langle\exp(i\vec{q}\cdot\vec{r}_0)\left|\frac{1}{r_{01}}+\frac{1}{r_{02}}-\frac{2}{r_0}\right|\exp(i\vec{k}_0\cdot\vec{r}_2)\right\rangle\left|\psi_i(\vec{r}_1,\vec{r}_2)\right\rangle,\quad \epsilon\to 0^+. \tag{3}$$

In the above expressions $\vec{r}_0$ is the coordinate of the incident electron, $\vec{r}_1$ and $\vec{r}_2$ refer to the coordinates of the initially bound electrons, and $r_{01}=|\vec{r}_0-\vec{r}_1|$, $r_{02}=|\vec{r}_0-\vec{r}_2|$. The quantity p^2 is given by $p^2=k_0^2-2\bar{w}$, $\bar{w}$ being the average excitation energy.[6] The helium ground-state wave function $\psi_i(\vec{r}_1,\vec{r}_2)$ which appears in Eqs. (2) and (3) was taken to be an analytical fit to the Hartree-Fock wave function, namely[8]

$$\psi_i(r_1,r_2)=\varphi_0(r_1)\varphi_0(r_2) \tag{4a}$$

with

$$\varphi_0(r)=(4\pi)^{-1/2}[A\exp(-\alpha r)+B\exp(-\beta r)] \tag{4b}$$

and $A=2.60505$, $B=2.08144$, $\alpha=1.41$, and $\beta=2.61$. For the final-state wave function $\psi_f(\vec{r}_1,\vec{r}_2)$ we used a symmetrized product of the He^+ ground-state wave function for the bound electron times a Coulomb wave $\varphi_{c,\vec{k}_B}{}^{Z=1}$ (corresponding to $Z=1$ and to an ejected-electron momentum $\vec{k}_B$) orthogonalized to the ground-state orbital φ_0. Thus

$$\psi_f(\vec{r}_1,\vec{r}_2)=2^{-1/2}[\varphi_{He^+ 1s}(r_1)\varphi_{c,\vec{k}_B}{}^{Z=1}(\vec{r}_2)+(1\leftrightarrow 2)], \tag{5a}$$

where

$$\varphi_{c,\vec{k}_B}{}^{Z=1}(\vec{r})=\psi_{c,\vec{k}_B}{}^{Z=1}(\vec{r})-\langle\varphi_0|\psi_{c,\vec{k}_B}{}^{Z=1}\rangle\varphi_0(r) \tag{5b}$$

and $\psi_{c,\vec{k}_B}{}^{Z=1}$ is a Coulomb wave corresponding to $Z=1$ and to the momentum $\vec{k}_B$.

Performing the integrals on the plane-wave parts of the matrix elements in Eq. (3), we find that

$$f_{SB2}=\frac{2}{\pi^2}\int d^3q\,\frac{1}{q^2-p^2-i\epsilon}\,\frac{1}{K_i^2K_f^2}\,\langle\psi_f(\vec{r}_1,\vec{r}_2)|[\exp(-i\vec{K}_f\cdot\vec{r}_1)+\exp(-i\vec{K}_f\cdot\vec{r}_2)-2]$$
$$\times[\exp(i\vec{K}_i\cdot\vec{r}_1)+\exp(i\vec{K}_i\cdot\vec{r}_2)-2]|\psi_i(r_1,r_2)\rangle, \tag{6}$$

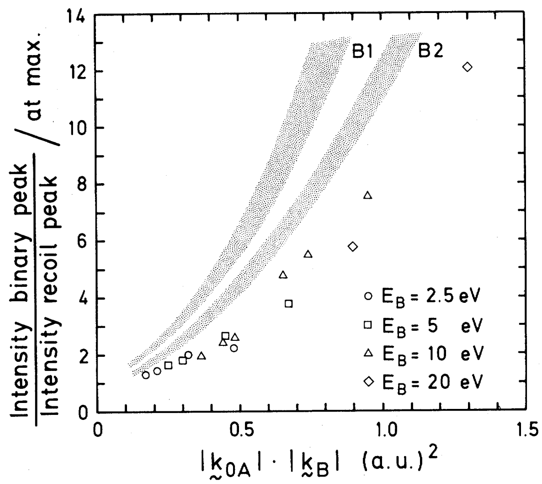

FIG. 4. The ratio of the intensity of the binary peak to that of the recoil peak, at the maximum, as a function of $|\vec{k}_{0A}|\,|\vec{k}_B|$, for $E_0=500$ eV. The experimental results are shown for $E_B=2.5$, 5, 10, and 20 eV. The first and second Born theoretical calculations, performed for $E_B=5$ and 10 eV, fall in the shaded areas indicated.

where $\vec{K}_i=\vec{k}_0-\vec{q}$ and $\vec{K}_f=\vec{k}_A-\vec{q}$. The expression (6) was evaluated numerically and the corresponding second Born-approximation results for the triply differential cross section were then obtained from Eq. (1). Figures 1 to 3 demonstrate that our second Born-approximation calculations yield very significant improvements over the first Born-approximation values. Indeed, the second Born-term results exhibit (i) a shift of the binary peak to larger angles than the direction of $\vec{k}_{0A}$ predicted by the first Born approximation (see Fig. 1); (ii) a shift of the recoil peak towards larger angles (see Figs. 1 and 2) than the direction $\vec{k}_{0A}$ predicted by the first Born approximation; (iii) a major enhancement of the magnitude of the recoil peak with respect to the value predicted by the first Born approximation. This last feature is dramatically illustrated in Fig. 3, where the ratio of the binary to the recoil peak is plotted as a function of the scattering angle θ_A, for $E_B=10$ eV. In Fig. 4 we also display this ratio as a function of the quantity $|\vec{k}_{0A}|\,|\vec{k}_B|$. This representation has the advantage of summarizing the results for different values of θ_A and E_B in a compact way.

It is clear from the above results that the theoretical treatment presented here accounts for all the key features of the experimental data. This strongly suggests that we have included all the relevant dynamical collision effects in our calculations. We believe that future theoretical work performed within the present dynamical framework should be able to account for the remaining discrepancies between theory and experiment by using more elaborate wave functions to describe both the helium ground state and especially the slowly ejected electron in the field of the ion.

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[1]H. Ehrhardt, K. H. Hesselbacher, K. Jung, and K. Willmann, in *Case Studies in Atomic Physics*, edited by E. W. McDaniel and M. R. C. McDowell (North-Holland, Amsterdam, 1972), Vol. 2, Chap. 3.

[2]E. Weigold and I. McCarthy, Phys. Rep. 27C, 275 (1976).

[3]E. Schubert, A. Schuck, K. Jung, and S. Geltman, J. Phys. B 12, 967 (1979).

[4]See, for example, V. L. Jacobs, Phys. Rev. A 10, 499 (1974); S. Geltman, J. Phys. B 7, 1994 (1974); W. D. Robb, S. P. Rountree, and T. Burnett, Phys. Rev. A 11, 1193 (1975); D. H. Madison, R. V. Calhoun, and W. N. Shelton, Phys. Rev. A 16, 552 (1977); B. H. Bransden, J. J. Smith, and K. H. Winters, J. Phys. B 11, 3095 (1978).

[5]F. W. Byron, Jr., and C. J. Joachain, Phys. Rev. A 8, 1267 (1973), and Phys. Rep. 34C, 233 (1977).

[6]C. J. Joachain, *Quantum Collision Theory* (North-Holland, Amsterdam, 1975), Chap. 19.

[7]F. W. Byron, Jr., C. J. Joachain, and B. Piraux, J. Phys. B 13, L673 (1980).

[8]F. W. Byron, Jr., and C. J. Joachain, Phys. Rev. 146, 1 (1966).