Coulomb interaction in the final state of electron impact ionization: Effects on the triple differential cross section

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An approach to the calculation of the impulsive $(e,2e)$ cross section, which extends the plane-wave-impulse approximation to include the long-range tails of the Coulomb interaction in the final state, is presented. The model divides the collision space into two regions: an inner sphere where short-range forces are active and responsible for the impulsive character of the collision, and an outer region where the tails of the Coulomb interactions act on the charged free particles, which can be treated in a semiclassical way. An extensive comparison between the predictions of this model and experimental data relative to atomic hydrogen and helium, as derived from the literature, is presented. The model constitutes an improvement over previous impulsive models, mainly for the angular distributions of $(e,2e)$ events.

I. INTRODUCTION

The study of $(e,2e)$ reactions has attracted growing interest since the first experiments[1-3] on the reaction mechanism and the spectroscopical applications. By an $(e,2e)$ reaction we mean an ionization process of an outer or inner shell of the target atom or molecule, induced by electron collision. This is, in principle, a many-body problem involving two free electrons plus a residual ion in the final state. Several attempts to produce models which fully describe these ionizing collisions have been made, and theory has developed along two lines, depending on the particular kinematics of the experiments.

For completely asymmetry conditions, where the final electrons have very different energies and emerging angles, first-Born-approximation theories were initially applied, with various modifications to include the residual interaction with the ion field (Coulomb-projected Born approximation), or electron correlation effects through the use of close-coupling and correlated wave functions for the target.[4-7] All of these models failed in predicting the position of the maxima in the angular distribution of the triple differential cross section and their intensity ratios, the backward scattering intensity being definitely underestimated. A many-body approach pointed at the importance of carefully choosing the scattering potentials and suggested that the shape of the angular distribution is sensitive to correlation between the outgoing electrons.[8] Distorted-wave calculations have also been performed, differences depending on the choice of the distorting potentials.[9-12] They generally achieved better agreement with the experiments than first-Born-approximation results. Recognition of the importance of consistently retaining higher terms in the Born series has also been done. A second Born treatment has shown the importance of second-order contributions to the $(e,2e)$ cross-section, both in the asymmetric regime, mainly for what concerns the backward lobe intensity, and in the symmetric one at very large scattering angles.[13] More recently the possibility to apply a first-order quantum-defect theory has also been considered.[14]

The symmetric kinematics of the $(e,2e)$ experiment involves even sharing of energy between the two final electrons. In the impulsive regime, when the incident energy is much higher than the binding energy of the target electron, the many-body problem can be reduced to a quasi-three-body scattering. A simple but effective approximation in this case has proved to be the plane-wave impulse approximation (PWIA), which allows for the $(e,2e)$ cross section being factorized in two terms: an electron-electron collision term, and the squared Fourier transform of the overlap between the initial atomic state and the final ionic one.[10] The good agreement with the experimental results is limited, however, to very high energies ($E \simeq 50$ times higher than the binding energy) and completely symmetric or nearly symmetric kinematics. Noticeable discrepancies found at lower energies and asymmetric conditions suggested the introduction of more sophisticated models. Formulations implying optical models for the free-electron wave functions lead to the fully factorized distorted-wave impulse approximation (DWIA).[10,15,16] Further approximation to the true optical potential introduces a constant complex potential [averaged eikonal-wave impulse approximation (EWIA)].[17,18] In this case the distorted waves of the free electrons are modified plane waves in the localized region relevant to the scattering event. Recently a completely different scheme to correct the PWIA has been proposed.[19] The ideas for this approach stem from the assumption that the impulsive ionizing process takes place within a small region of space, whose radius r_0 is determined by the wave function of the orbital involved in the reaction. This region is the crucial one for the dynamics of the process and is responsible for the short-range behavior of the scattering potentials. Within this domain the $(e,2e)$ amplitude can be calculated and factorized as in PWIA. In the outer region

the mutual repulsion between the final electrons is taken into account. The two electrons are treated as semiclassical particles moving in a Coulomb field, due to the interaction with the residual ion and with each other. As a result their trajectories are deflected and the change of momentum suffered by the electrons will affect the differential cross section. The purpose of this work is to calculate, on the basis of this approach [plane-wave impulse approximation plus semiclassical correction (PWIA-SC)], the triple differential cross section for the ionization of H and He.

General outlines of the theory are given in Sec. II and atomic units will be used throughout the paper. In Sec. III the results of the calculation are compared with completely symmetric, energy-sharing, asymmetric experimental data and with previous calculations. Section IV is devoted to comments on the present results and to limits and possible extensions of the model.

II. THEORY

Under kinematic conditions which are characteristic of "impulsive" ionization, i.e., large energy and momentum transfer as compared to the binding energy and momentum of the struck electron, the many-body problem of the reaction

$$e^- + A \rightarrow e_1^- + e_2^- + A^+$$

can be reduced to a three-body one.

If the vectors $\mathbf{x}_1=(\mathbf{r}_1,\sigma_1)$ and $\mathbf{x}_2=(\mathbf{r}_2,\sigma_2)$ describe the position and the spin state of the two outgoing electrons in the field of the infinitely massive nucleus, we can write the three-body time-independent Schrödinger equation as

$$(E-H_{10}-H_{20}-V_1-V_2-V_{12})\langle \mathbf{x}_1\mathbf{x}_2 \mid \psi\rangle = 0 \ . \tag{1}$$

The free Hamiltonian is given by

$$H_{10}+H_{20} = -\frac{\partial^2}{\partial \mathbf{r}_1^2} - \frac{\partial^2}{\partial \mathbf{r}_2^2} \ .$$

V_i, $i=1,2$, is the field seen by the free electron in presence of the atomic system. The averaged Hartree-Fock field will be assumed:

$$V_i(r_i) = -\frac{Z(r_i)}{r_i}, \quad i=1,2 \tag{2}$$

$$Z(r_i) = N - r_i \sum_{n\lambda,\sigma_i} c_{n\lambda} \int \varphi^*_{n\lambda}(\mathbf{x}_i') \frac{d\mathbf{r}_i'}{|\mathbf{r}_i-\mathbf{r}_i'|} \varphi_{n\lambda}(\mathbf{x}_i') \ . \tag{3}$$

N is the nuclear charge and the summation is done over the totality of filled-up spin orbitals $\varphi_{n\lambda}(\mathbf{x})$, whose occupation number is $c_{n\lambda}$. This is a reasonable assumption when both of the outgoing particles are fast enough and the residual ion behaves like a spectator during the reaction time. Finally, V_{12} is the electron-electron interaction

$$V_{12} = \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} \ . \tag{4}$$

The formal derivation of the wave function in (1) should consider the explicit expansion

$$\langle \mathbf{x}_1\mathbf{x}_2 \mid \psi\rangle = \mathscr{A}\langle \mathbf{r}_1\mathbf{r}_2 \mid \psi\rangle\langle \sigma_1\sigma_2 \mid \chi\rangle \ ,$$

where $|\psi\rangle$ and $|\chi\rangle$ are, respectively, the orbital and spin-wave functions, and $\mathscr{A}$ implies fully antisymmetrization. In the nonrelativistic approximation the interaction of charged particles does not depend on their spin. The Schrödinger equation (1) determines the orbital wave function only, while leaving $|\chi\rangle$ undetermined and factorized out. To avoid redundancy the explicit spin dependence of the wave functions will be omitted throughout the derivation. The effect of the identity of the particles will be finally taken into account in the derivation of the cross section.

Equation (1) can be reduced to the proper Faddeev equations for independent systems of two particles in an external field.[20] Let us put

$$|\psi\rangle = |\psi_{12}\rangle + |\psi_{(1,2)}\rangle \ , \tag{5}$$

where $|\psi_{12}\rangle$ is the wave function of two particles interacting with each other through the potential V_{12}, while $|\psi_{(1,2)}\rangle$ is the wave function of the system of two light particles in the field of a third infinitely massive nucleus when $V_{12}=0$. These wave functions satisfy the following set of coupled equations:

$$\begin{aligned} &(E-H_{10}-H_{20})\,|\psi_{12}\rangle = V_{12}\,|\psi\rangle \ , \\ &(E-H_{10}-H_{20})\,|\psi_{(1,2)}\rangle = (V_1+V_2)\,|\psi\rangle \ , \end{aligned} \tag{6}$$

E being the total energy of the system. They are expressed in terms of the total Green's function as

$$\begin{aligned} &|\psi_{12}\rangle = \hat{G}_{12}(E)V_{12}\,|\psi_{(1,2)}\rangle \ , \\ &|\psi_{(1,2)}\rangle = \hat{G}_{(1,2)}(E)(V_1+V_2)\,|\psi_{12}\rangle + |\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle \end{aligned} \tag{7}$$

with the usual definitions

$$\begin{aligned} &\hat{G}_{12}(E) = (E-H_{10}-H_{20}-V_{12}+i0)^{-1} \ , \\ &\hat{G}_{(1,2)}(E) = (E-H_{10}-H_{20}-V_1-V_2+i0)^{-1} \ . \end{aligned} \tag{8}$$

$|\varphi_{01}\rangle$ and $|\varphi_2(\mathbf{p}_0)\rangle$ are single-particle states, solutions of the following Schrödinger equations:

$$\begin{aligned} &(\epsilon_{n\lambda}-H_{10}-V_1)\,|\varphi_{01}\rangle = 0 \ , \\ &(E_0-H_{20}-V_2)\,|\varphi_2(\mathbf{p}_0)\rangle = 0 \ , \end{aligned} \tag{9}$$

$\epsilon_{n\lambda}$ and E_0 are bound and continuum single-particle energies, $\mathbf{p}_0$ is the initial momentum of the projectile. By using the well known relation $\hat{G}_i V_i = \hat{G}_0 t_i$, the set of equations (7) can be written in the following form:

$$\begin{aligned} &|\psi_{12}\rangle = \hat{G}_0(E)t_{12}(E)\,|\psi_{(1,2)}\rangle \ , \\ &|\psi_{(1,2)}\rangle = \hat{G}_0(E)\tau_{12}(E)\,|\psi_{12}\rangle + |\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle \ , \end{aligned} \tag{10}$$

where $\hat{G}_0(E)$ is the free Green's function

$$\hat{G}_0(E) = (E-H_{10}-H_{20}+i0)^{-1} \tag{11}$$

and the new scattering operators are defined as[20]

$$t_{12}(E)=V_{12}+V_{12}\hat{G}_0(E)t_{12}(E)\ ,$$
$$\tau_{12}(E)=(V_1+V_2)+(V_1+V_2)\hat{G}_0(E)\tau_{12}(E)\ . \tag{12}$$

It can be shown that τ_{12} has the following main feature:

$$[1+\hat{G}_0\tau_{12}(E)]\,|\,\mathbf{p}_1\mathbf{p}_2\rangle=|\,\varphi_1(\mathbf{p}_1)\varphi_2(\mathbf{p}_2)\rangle\ , \tag{13}$$

and acts on the plane waves as a distorting operator. The formal solution of equations (7) can now be written in serial form

$$|\,\psi\rangle=|\,\psi_{12}\rangle+|\,\psi_{(1,2)}\rangle=|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle +\hat{G}_0(E)\Phi(E)t_{12}\,|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle\ , \tag{14}$$

where

$$\Phi(E)=1+T(E)\hat{G}_0(E)\ , \tag{15}$$

$$T(E)=\tau_{12}+t_{12}\hat{G}_0\tau_{12}+\tau_{12}\hat{G}_0t_{12}\hat{G}_0\tau_{12}+\cdots\ . \tag{16}$$

Let us stop the series to the first term, i.e., $T(E)=\tau_{12}(E)$. The following expression is obtained:

$$|\,\psi\rangle=|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle+\hat{G}_0(1+\tau_{12}\hat{G}_0)t_{12}\,|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle \tag{17}$$

or, in coordinate representation,

$$\langle\,\mathbf{r}_1\mathbf{r}_2\,|\,\psi\rangle =\varphi_{01}(\mathbf{r}_1)\varphi_2(\mathbf{r}_2,\mathbf{p}_0) +\frac{1}{(2\pi)^6}\int d^3p_1'd^3p_2'\frac{e^{i\mathbf{p}_1'\cdot\mathbf{r}_1+i\mathbf{p}_2'\cdot\mathbf{r}_2}}{E-p_1'^2-p_2'^2+i0} \times\langle\,\mathbf{p}_1\mathbf{p}_2\,|\,(1+\tau_{12}G_0)t_{12}\,|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle\ . \tag{18}$$

To get the value of the ionization cross section the limit $r_1,r_2\to\infty$ should be taken. Let us use Jacobian coordinates in a six-dimensional space so as to have $r_1=\rho\cos\alpha$ and $r_2=\rho\sin\alpha$ ($\alpha\neq0$) with $\rho\to\infty$. In this case, by using the stationary phase method, the asymptotic wave function is written

$$\langle\,\mathbf{r}_1\mathbf{r}_2\,|\,\psi\rangle_{\rho\to\infty}\simeq\frac{(-2i\sqrt{E}\,)^{3/2}}{(32\pi)^{5/2}}\frac{\exp(i\sqrt{E}\,\rho)}{\rho^{5/2}}T_0(\mathbf{p}_0;\mathbf{p}_1,\mathbf{p}_2)\ , \tag{19}$$

where

$$T_0(\mathbf{p}_0;\mathbf{p}_1,\mathbf{p}_2)=\langle\,\mathbf{p}_1\mathbf{p}_2\,|\,(1+\tau_{12}\hat{G}_0)t_{12}\,|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle \tag{20}$$

and $\mathbf{p}_i=\sqrt{E}\,\mathbf{r}_i/\rho$, i.e., $(p_1^2+p_2^2)=E$. By using the equation (13), the term T_0 assumes the following expression:

$$T_0(\mathbf{p}_0;\mathbf{p}_1,\mathbf{p}_2)=\langle\,\varphi_1(\mathbf{p}_1)\varphi_2(\mathbf{p}_2)\,|\,t_{12}\,|\,\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle\ , \tag{21}$$

which is the matrix element of the ionization process we are looking for. It is the most complete expression of a first-order approximation with respect to t_{12}. Any less crude approximation should include t_{12} at least twice or more. The formula (19) can, indeed, be taken as the common starting point for most of those calculations which consider the distortion effect due to the presence of an ion field as the main feature to be accounted for. When the ion field is completely neglected, plane waves are used for both the incident and outgoing particle (PWIA). In the Coulomb-projected Born approximation the slow electron is described by a Coulomb wave and the scattering operator t_{12} is replaced by the potential V_{12}. The EWIA introduces distortion through an averaged optical potential well, which modifies the plane waves by simply shifting their wave numbers.

The main problem arising within this approach is for the function $\langle\,\mathbf{r}_1\mathbf{r}_2\,|\,\psi\rangle$ in (18) to have the wrong asymptotic behavior; we lose information about the correlation of electrons due to rescattering and are faced with the divergencies of integrals as soon as we want to calculate higher-order approximations. Furthermore, due to the long-range tail of the Coulomb potential, there is a noncentral mutual interaction of the free electrons in the final state, which should result in a non-negligible effect on the cross section. Partial account of it has already been attempted,[19,21] and the discrepancies observed between first-Born-approximation calculations and $(e,2e)$ experiments on hydrogen were reduced. This result prompted us to move further along this way and to develop the quantum-mechanical treatment which is presented in the following.

The basic idea can be found in the paper of Presniakov[22] and has been recently developed by Popova and Popov[20] and Mukhamedzhanov *et al.*[23] It consists in dividing the space into two regions: an inner one of radius r_0, where the system undergoes the quantum-mechanical transition under the effect of short-range interactions; an outer region where the system evolves asymptotically in the presence of the long-range tail of the Coulomb potentials. A suitable mathematical frame to treat this problem can be found in the paper of Merkuriev.[24] Let us write the full interaction responsible for the $(e,2e)$ impulsive reaction as a sum of two terms; the first one responsible for the short-range character of the forces, and the second one including the long-range part of the Coulomb potentials. By means of the usual step function

$$\Theta(r_i-r_j)=\begin{cases}0, & r_i<r_j\\ 1, & r_j\le r_i\end{cases}$$

the following potential terms can be defined:

$$V_i^{\rm in}=V_i\Theta(r_0-r_i),\quad V_{ij}^{\rm in}=V_{ij}\Theta(r_0-r_i)\Theta(r_0-r_j)\ ,$$
$$V_i^{\rm out}=V_i\Theta(r_i-r_0),\quad V_{ij}^{\rm out}=V_{ij}\Theta(r_i-r_0)\Theta(r_j-r_0)\ . \tag{22}$$

$V^{\rm in}$ is active in the inner region only, while $V^{\rm out}$ is active outside the sphere. Following this notation the Hamiltonian H_0^c can be defined as

$$H_0^c = H_{10} + H_{20} + V_1^{\text{out}} + V_2^{\text{out}} + V_{12}^{\text{out}} , \tag{23}$$

which coincides with the free Hamiltonian of two electrons for $r_1, r_2 < r_0$. The Schrödinger equation (1) becomes

$$(E - H_0^c - V_1^{\text{in}} - V_{12}^{\text{in}}) \langle \mathbf{r}_1 \mathbf{r}_2 \mid \psi \rangle = 0 . \tag{24}$$

By using the new Green's function $\hat{G}_0^c = (E - H_0^c + i0)^{-1}$ instead of $\hat{G}_0$, all of the previously obtained results can be reproduced. The following formula is equivalent to (14):

$$\mid \psi \rangle = \mid \varphi_0(\mathbf{p}_0) \rangle + \hat{G}_0^c(E) \Phi^c(E) t_{12}^c \mid \varphi_0(\mathbf{p}_0) \rangle , \tag{25}$$

$$\Phi^c(E) = [1 + T^c(E) \hat{G}_0^c(E)] ,$$

$$T^c(E) = \tau_{12}^c + t_{12}^c G_0^c \tau_{12}^c + \tau_{12}^c G_0^c t_{12}^c G_0^c \tau_{12}^c + \cdots , \tag{26}$$

and the two scattering operators τ_{12}^c and t_{12}^c are determined by the Lippmann-Schwinger equations analogous to (12),

$$t_{12}^c = V_{12}^{\text{in}} + V_{12}^{\text{in}} G_0^c t_{12}^c ,$$

$$\tau_{12}^c = (V_1^{\text{in}} + V_2^{\text{in}}) + (V_1^{\text{in}} + V_2^{\text{in}}) G_0^c \tau_{12}^c . \tag{27}$$

V^{in}'s are now short-range potentials. The boundary condition $\mid \varphi_0(\mathbf{p}_0) \rangle$ is a solution of the following equation:

$$(E - H_{10} - H_{20} - V_1 - V_2 - V_{12}^{\text{out}}) \mid \varphi_0(\mathbf{p}_0) \rangle = 0 , \tag{28}$$

and only if we neglect V_{12}^{out} does $\mid \varphi_0(\mathbf{p}_0) \rangle = \mid \varphi_{01} \varphi_2(\mathbf{p}_0) \rangle$. By limiting the series (26) to the first term $T^c = \tau_{12}^c$ (first order in t_{12}^c), it follows that

$$\mid \psi \rangle = \mid \varphi_0(\mathbf{p}_0) \rangle + G_0^c (1 + \tau_{12}^0 G_0^c) t_{12}^c \mid \varphi_0(\mathbf{p}_0) \rangle . \tag{29}$$

Asymptotically, beyond the domain of short-range forces, i.e., for $r_1, r_2 > r_0$, the equation (24) becomes

$$(E - H_0^c) \mid \psi \rangle = 0 \tag{30}$$

with the boundary condition

$$\langle \mathbf{r}_1, \mathbf{r}_2 \mid \psi \rangle = \langle \mathbf{r}_1, \mathbf{r}_2 \mid G_0^c (1 + \tau_{12}^c G_0^c) t_{12}^c \mid \varphi_0(\mathbf{p}_0) \rangle ,$$

$$r_1, r_2 = r_0 . \tag{31}$$

In the case of symmetric or nearly symmetric $(e,2e)$ experiments at incident energies E_0 of hundreds of eV and for outermost orbitals, the following relationships, on which first-order approximations rely, are usually fulfilled:

$$\frac{\epsilon_{n\lambda}}{E_i} \ll 1, \quad \frac{1}{E_{12} r_0} \ll 1, \quad \sqrt{E_i} r_0 \gg 1 . \tag{32}$$

E_i is the kinetic energy of the outgoing electrons and E_{12} is their relative energy. Under these conditions, the potentials being weak and slowly varying over distances comparable to the wavelength $\lambda_i = 1/k_i$, the Schrödinger equation in the outer region can be solved semiclassically by making the approximations of geometrical optics. A solution is sought for equation (30) in the form

$$\langle \boldsymbol{\rho} \mid \psi \rangle = \frac{(-2i\sqrt{E})^{3/2}}{(32\pi)^{5/2}} A(\boldsymbol{\rho}) e^{i\chi(\boldsymbol{\rho})} . \tag{33}$$

Under this ansatz the amplitude A and the eikonal function χ satisfy differential equations

$$(\nabla_\rho \chi)^2 = E - V_1^{\text{out}} - V_2^{\text{out}} - V_{12}^{\text{out}} , \tag{34}$$

$$\text{div}_\rho (A^2 \nabla_\rho \chi) = 0 . \tag{35}$$

The relationship (34) corresponds to a set of characteristic equations which determine the trajectories $\boldsymbol{\rho}(t) = \{\mathbf{r}_i(t)\}$ of the electrons in the outermost region. t is a parameter to which the meaning of time can be attributed. If $r_i(0) = r_0$ is chosen, then $r_i(\infty)$ is the coordinate of ith electron at the detector. The solution of Eq. (34), under validity of the relations (32), was done in Refs. 19 and 25. Classical paths are derived and the effect of the residual Coulomb interactions to the first order is shown to result in a deflection $\Delta\theta_i$ of the free electrons from the straight line. The amplitude $A(\boldsymbol{\rho})$ is obtained from Eq. (35). Let us write

$$\nabla_\rho \chi = n(\boldsymbol{\rho}) \mathbf{l}, \quad n(\boldsymbol{\rho}) = (E - V_1^{\text{out}} - V_2^{\text{out}} - V_{12}^{\text{out}})^{1/2} , \tag{36}$$

$\mathbf{l}$ being the unitary vector tangent to the curve $\boldsymbol{\rho}(t)$. The Gauss theorem allows us to write

$$\int_V \text{div}_\rho (n A^2 \mathbf{l}) dV = \oint_\Sigma n A^2 \mathbf{l} \cdot \mathbf{m} \, d\sigma , \tag{37}$$

where Σ can be chosen as the surface of a small tube parallel to the electron rays, delimited by squares $d\sigma_1, d\sigma_2$ of eikonal surfaces $\chi_1 = \text{const}$ and $\chi_2 = \text{const}$. Then it is $n A^2 d\sigma = \text{const}$, which is no more than the energy conservation law, and

$$A^2(t) = A^2(0) \frac{n(0)}{n(t)} \frac{d\sigma(0)}{d\sigma(t)} . \tag{38}$$

For spherical eikonal surfaces in a six-dimensional space, it is $d\sigma(0)/d\sigma(t) = \rho_0^5/\rho^5(t)$. $A^2(t)$ is evaluated along the classical paths of electrons, i.e., if $A^2(0) = A^2(\theta_1, \theta_2)$ then $A^2(\infty) = A^2(\theta_1 + \Delta\theta_1, \theta_2 + \Delta\theta_2)$.

As the last step, the amplitude $A(0)$ is to be determined and matched with the wave function (31). Let us first neglect the effects of the Coulomb tails in (31) and assume that for rather big energies the asymptotic expression (19) is valid at $r_1, r_2 = r_0$. The presence of the Coulomb tails in the external region will produce a reflected spherical wave. It will be

$$\langle \mathbf{r}_1, \mathbf{r}_2 \mid \psi \rangle \simeq \frac{(-2i\sqrt{E})^{3/2}}{(32\pi)^{5/2}} \left[T_0(\mathbf{p}_0; \mathbf{p}_1, \mathbf{p}_2) \frac{\exp(i\sqrt{E}\rho)}{\rho^{5/2}} + \gamma \frac{\exp(-i\sqrt{E}\rho)}{\rho^{5/2}} \right] . \tag{39}$$

By matching the expression (39) with the eikonal one, (33), it is found that

$$A(0) = 2 \frac{T_0(\mathbf{p}_0; \mathbf{p}_1, \mathbf{p}_2)}{\rho_0^{5/2} [1 + n(0)/n(\infty)]} \tag{40}$$

and then

$$\langle \mathbf{r}_1,\mathbf{r}_2 \mid \psi \rangle_{\rho\to\infty} \simeq \frac{(-2i\sqrt{E})^{3/2}}{(32\pi)^{5/2}} \times \frac{T_0(\mathbf{p}_0;\mathbf{p}_1(\infty),\mathbf{p}_2(\infty))F(n(0)/n(\infty))}{\rho^{5/2}} \times \exp[i\sqrt{E}\rho - i\nu\ln(2\sqrt{E}\rho)] , \quad (41)$$

where

$$F(x)=2\sqrt{x}/(1+x) , \qquad \nu=-\frac{1}{2}\left[\frac{1}{p_1}+\frac{1}{p_2}-\frac{1}{|\mathbf{p}_1-\mathbf{p}_2|}\right] . \quad (42)$$

$T_0(\mathbf{p}_0;\mathbf{p}_1(\infty),\mathbf{p}_2(\infty))$ differs from $T_0(\mathbf{p}_0;\mathbf{p}_1,\mathbf{p}_2)$ in (19) because of the angular shifts $\Delta\theta_i$ suffered by the free electrons along their paths in the external region. It has to be noted that the wave function in (41) now has the correct asymptotic behavior.

The calculation of the cross section implies the usual average over the spin states of two identical particles system. That means that the triple differential cross section will be expanded in the following terms:

$$\frac{d^3\sigma}{dE\,d\omega_1 d\omega_2} \propto [\,|\,T_0(\mathbf{p}_0;\mathbf{p}_1(\infty),\mathbf{p}_2(\infty)) + T_0(\mathbf{p}_0;\mathbf{p}_2(\infty),\mathbf{p}_1(\infty))\,|^2 + 3\,|\,T_0(\mathbf{p}_0;\mathbf{p}_1(\infty),\mathbf{p}_2(\infty)) - T_0(\mathbf{p}_0;\mathbf{p}_2(\infty),\mathbf{p}_1(\infty))\,|^2] . \quad (43)$$

If the plane-wave impulse approximation is adopted to calculate the scattering amplitude T_0, then the scattering cross section is finally written as

$$\frac{d^3\sigma}{d\omega_1 d\omega_2 dE} = C\left[\frac{d^3\sigma(\theta_1-\Delta\theta_1,\theta_2-\Delta\theta_2,\varphi)}{d\omega_1 d\omega_2 dE}\right]_{\text{PWIA}} ,$$

where

$$\left[\frac{d^3\sigma}{d\omega_1 d\omega_2 dE}\right]_{\text{PWIA}} = 4\frac{p_1 p_2}{p_0} f_t g(\mathbf{q}) , \quad (45)$$

$$f_t=\frac{2\pi\eta}{\exp(2\pi\eta)-1}\left\{\frac{1}{|\mathbf{P}'-\mathbf{P}|^4}+\frac{1}{|\mathbf{P}'+\mathbf{P}|^4}-\frac{1}{|\mathbf{P}'-\mathbf{P}|^2}\frac{1}{|\mathbf{P}'+\mathbf{P}|^2}\cos\left[\eta\ln\left[\frac{|\mathbf{P}'+\mathbf{P}|^2}{|\mathbf{P}'-\mathbf{P}|^2}\right]\right]\right\} ,$$

$$\eta=\frac{1}{2P'} , \quad \mathbf{P}=\tfrac{1}{2}(\mathbf{p}_0+\mathbf{q}) , \quad \mathbf{P}'=(\mathbf{p}_1-\mathbf{p}_2) . \quad (46)$$

f_t is the e-e factor[17] calculated on the basis of the t matrix. $\mathbf{q}$ is the recoil momentum defined by the relationship $\mathbf{p}_0+\mathbf{q}=\mathbf{p}_1+\mathbf{p}_2$, while $g(\mathbf{q})$ is the squared Fourier transform of the overlap of the initial atomic state with the final ionic one. The angles θ_i and θ_2 are the angles formed by $\mathbf{p}_1$ and $\mathbf{p}_2$ with the projection of $\mathbf{p}_0$ in the plane of $\mathbf{p}_1$ and $\mathbf{p}_2$. φ is then the azimuthal angle of $\mathbf{p}_0$. The analytical expression for the angular deflection is

$$\Delta\theta_i=\frac{1}{E_i r_0}\frac{p_i\cos(\alpha_0/2)[\,|\mathbf{p}_1-\mathbf{p}_2|+2p_j\sin(\alpha_0/2)]}{4\,|\mathbf{p}_1-\mathbf{p}_2|\sin(\alpha_0/2)[\,|\mathbf{p}_1-\mathbf{p}_2|+(p_1+p_2)\sin(\alpha_0/2)]} \quad (47)$$

while the coefficient C is given by

$$C=\frac{4a^2}{(1+a^2)^2} , \qquad a^2=1+\frac{2}{E_0 r_0}\left[Z_i(r_0)-\frac{1}{4\sin(\alpha_0/2)}\right] , \qquad \alpha_0=\theta_1+\theta_2 . \quad (48)$$

III. RESULTS

The differential cross section calculated by the present model (PWIA-SC) is compared with experimental data relative to atomic hydrogen and helium as derived from the literature. The results of various impulsive calculations are also presented. They are the simple PWIA, the EWIA, and, when data are available in the literature, the fully distorted-wave DWIA.

Atomic hydrogen is the best target in order to test the ionization reaction mechanism. Nevertheless, comparison with helium is important because of the very large body of experimental results available for this atom. Moreover, He $(e,2e)$ cross sections are known on an absolute scale in the impulsive kinematic regime, which is of interest for the present study.

It has to be pointed out that the radius r_0 is the only free parameter of the theory. In the case of He its value has been determined by fitting the completely symmetric coplanar cross section as measured at 424.5 eV incident energy.[18,26] The best fit to the experimental data is achieved for $r_0=0.70a_0$, a_0 being the Bohr radius. It is very close to the mean radius calculated from the Hartree-Fock He(1s) orbital of Clementi and Roetti[27] ($r_0=0.67a_0$). The derived value has been used throughout the calculations to predict the $(e,2e)$ cross section for all of the kinematical conditions examined. They are

(i) absolute determination of the cross section in a com-

pletely symmetric geometry, at scattering angles close to 45° and variable incident energy;

(ii) angular distributions taken in a completely symmetric geometry for various incident energies;

(iii) energy-sharing experiments;

(iv) angular distributions taken in coplanar asymmetric geometry fulfilling the condition of constant recoil momentum.

The PWIA-SC predictions are first compared with the absolute determination of the $(e,2e)$ cross section at different energies [condition (i)]. Reliable absolute experimental data exist for symmetric geometry at 45° scattering angles and 200–2800 eV incident energy.[28] They are reported in Fig. 1 together with the other available set of experimental data[29] and with the calculations. The agreement is noticeable all over the curve except for the point at the lowest energy which is definitely overestimated by the PWIA-SC. In the region of recoil momentum $q \simeq 0$ explored by these data, the EWIA, which uses the depth of the distorting potential well as a free parameter, gives better predictions in the lower energy range.

When angular distributions are measured for condition (ii), the kinematical conditions are widely changed. At 200 eV incident energy, recoil momenta up to $q=1.4a_0^{-1}$ are involved. In Fig. 2 two different determinations[30,31] of the angular distribution in coplanar symmetry reaction are reported together with calculations. The relative experimental cross sections are brought to absolute scale by scaling the value at 45° to the measured absolute value.[28] Full agreement is achieved by the present theory for what concerns the shape of the distribution, even at scattering

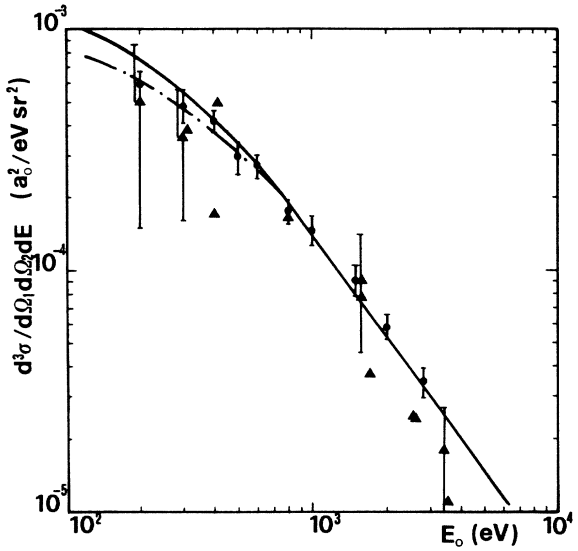

FIG. 1. The He coplanar symmetric $(e,2e)$ cross section at 45° scattering angle, plotted as a function of the incident energy. Experimental data are those of van Wingerden *et al.*, Ref. 28 (●), and of Stefani *et al.*, Ref. 29 (▲). Solid curve is the present PWIA-SC result, the dotted-dashed curve is the EWIA ($\bar{V}=20$ eV).

angles lower than 40°. The absolute value is, however, overestimated by a factor 1.3. None of the other models correctly account for the angular shape in this region, where the correlation effects between the final electrons

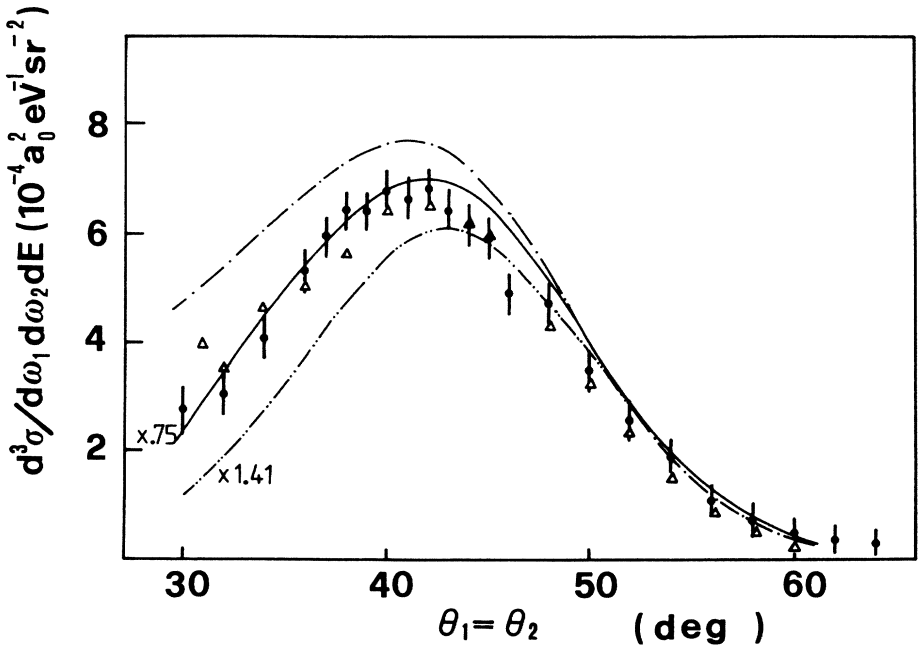

FIG. 2. The He $(e,2e)$ angular correlation measured at 200 eV incident energy and coplanar symmetric kinematics. The measured cross sections of Camilloni *et al.*, Ref. 30 (●), and of Fuss *et al.*, Ref. 31 (△), are compared with theoretical predictions of the present PWIA-SC (——), and EWIA ($\bar{V}=20$ eV) (—·—). (—··—) is the DWIA, as calculated by Fuss *et al.*, Ref. 31. Normalization of the relative experimental data has been done by scaling the value at 45° to the measured absolute cross section of van Wingerden *et al.*, Ref. 28.

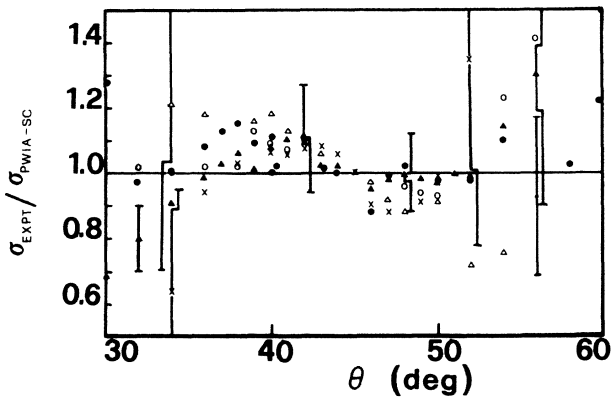

FIG. 3. The ratio $\sigma_{expt}/\sigma_{theor}$ between the measured $(e,2e)$ cross section and the theoretical value, calculated in the present PWIA-SC, is plotted vs the scattering angle $\theta=\theta_1=\theta_2$ for symmetric coplanar reactions at 200 (●), 400 (▲), 800 (○), 1600 (△), and 2500 eV (×) incident energy. The experimental data are those of Camilloni *et al.*, Ref. 30, and have been normalized to the PWIA-SC value at 45°.

are expected to be relevant. The more sophisticated DWIA (Ref. 31) lies below the experiment over the whole angular range, underestimating the absolute value of the cross section by a factor 1.4 at the larger scattering angles ($\theta \geq 50°$) and by a factor of 2.8 at small angles ($\theta=30°$). The agreement of PWIA-SC improves rapidly as the energy increases and at 400 eV even the absolute value is well reproduced all over the distribution. The results of comparison for several different energies are summarized in Fig. 3, where the ratio between experimental data and theory is shown as a function of the scattering angle. The experimental data have been normalized to the PWIA-SC value at 45°. Normalization factors range from 0.75 to 1.1. Disregarding the extreme angular regions, where uncertainties in the experimental data are large, the measurements are always within ±15% with respect to the theory.

Recently, two experiments in energy-sharing (iii) conditions have been reported.[26,32] In these experiments the incident energy and scattering angles are kept fixed, while the final kinetic energy is unevenly shared between the emerging electrons. In Table I the results of Stefani and Camilloni[26] are reported together with the predictions of the PWIA-SC, PWIA, and EWIA. The asymmetric kinematics explored by the experiment are still impulsive and the presence of any correlation between the two free electrons, should be evinced by the semiclassical correction, which in fact achieves better agreement with the data than the other impulsive approximations at low relative scattering angles.

The most interesting situation in regard to checking the predictions of the present model is represented by the coplanar asymmetric geometry, in which the recoil momentum q is kept almost constant [condition (iv)]. In these re-

TABLE I. The experimental and theoretical $(e,2e)$ cross section on He, relative to coplanar energy-sharing geometry and $\theta=\theta_1=\theta_2$ at 424.5 eV incident energy. Relative experimental data by Ref. 26 are reported together with theoretical predictions of PWIA-SC, PWIA, and EWIA. Experimental uncertainties are given in parentheses as one-standard-deviation error. Both the calculations and experiment have been normalized to the completely symmetric value at 45°, taken as 1.00.

θ	E_1 (eV)	E_2 (eV)	Expt.[a]	PWIA-SC	PWIA	EWIA[b]
35°	200	200	0.50(0.07)	0.51	0.85	0.57
	220	180	0.48(0.07)	0.48	0.80	0.55
	240	160	0.35(0.05)	0.40	0.66	0.47
	260	140	0.25(0.04)	0.31	0.49	0.37
	270	130	0.20(0.04)	0.26	0.40	0.31
	280	120	0.12(0.03)	0.21	0.32	0.26
	300	100	0.14(0.03)	0.13	0.19	0.17
45°	200	200	1.00(0.05)	1.00	1.00	1.00
	210	190	0.91(0.11)	0.96	0.96	0.94
	220	180	0.87(0.08)	0.86	0.87	0.88
	230	170	0.68(0.07)	0.72	0.73	0.74
	240	160	0.54(0.08)	0.56	0.58	0.60
	250	150	0.40(0.05)	0.40	0.43	0.48
	260	140	0.22(0.04)	0.30	0.31	0.35
	280	120	0.12(0.02)	0.14	0.15	0.17
	300	100	0.04(0.01)	0.06	0.06	0.08
50°	200	200	0.46(0.03)	0.48	0.39	0.46
	230	170	0.30(0.03)	0.34	0.28	0.33
	260	140	0.09(0.01)	0.13	0.12	0.16
	280	120	0.05(0.01)	0.06	0.06	0.07

[a]Stefani and Camilloni, Ref. 26.
[b]Calculated for $\bar{V}=20$ eV, Ref. 18.

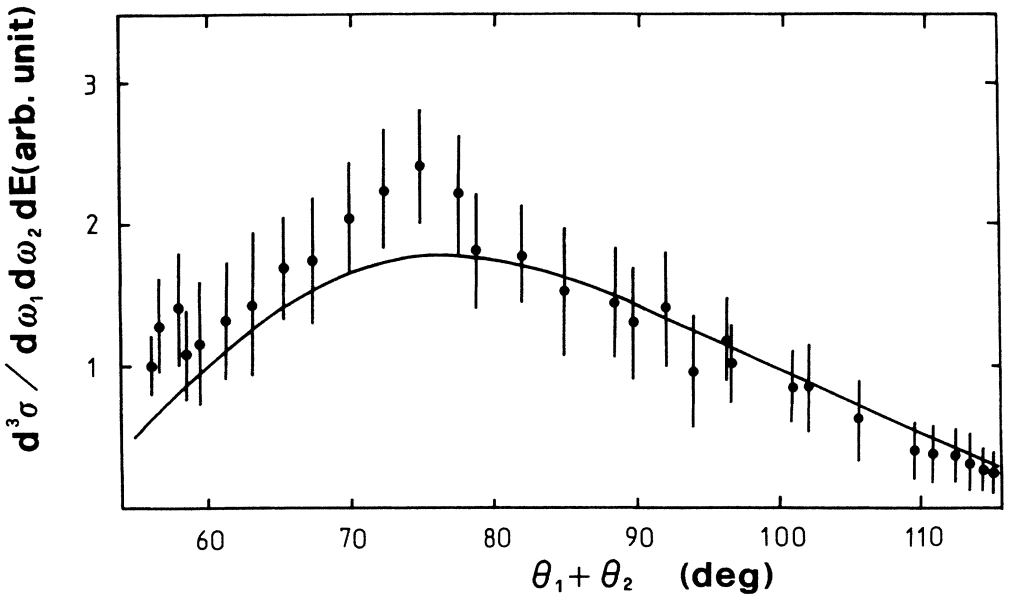

FIG. 4. The He $(e,2e)$ cross section relative to the coplanar asymmetric geometry, where $E_1 = E_2$, $\theta_1 \neq \theta_2$ and $q \simeq \cos t = 1.0 a_0^{-1}$. The data of Camilloni *et al.*, Ref. 33, are relative to 215 eV incident energy. The solid curve is the present PWIA-SC prediction. The relative experimental data have been normalized to the theoretical value at the largest scattering angle.

actions[18,33] the condition $E_1 = E_2$ is always maintained while the angles θ_1, θ_2 are properly varied. In this situation the behavior of the cross section is expected to be determined by the *e-e* factor, the form factor being constant. Experiments were performed at 215, 409, and 790 eV incident energies and the relative angle between the final electrons was varied from 56° to 110°. In Fig. 4 comparison is explicitly presented for the experiment at the lowest energy, while the global trend of the ratio of experimental to theoretical values is shown in Fig. 5. The experimental data have been normalized in both figures to the PWIA-SC value at the largest scattering angle. The *e-e* factor, as calculated in the present model, is fairly good even at energies as low as 215 eV and angles $\theta_1 + \theta_2 \leq 70°$. This fact represents an improvement with respect to the EWIA, which has already failed in fitting the experimental data at 400 eV incident energy and scattering angles smaller than 70°.[18] At higher energies the full body of experimental results agrees within ±20% with PWIA-SC predictions.

As concerns hydrogen, the semiclassical correction has been applied by choosing the value $r_0 = 1$. a_0 is used for the free parameter, as suggested by the result obtained for He. The experimental data are from measurements by Weigold *et al.*[10] in coplanar angular symmetry (Fig. 6) and asymmetric (Fig. 7) conditions, at 413.6 eV incident energy. The improvement achieved by the present model over the simple PWIA and the DWIA is evident in

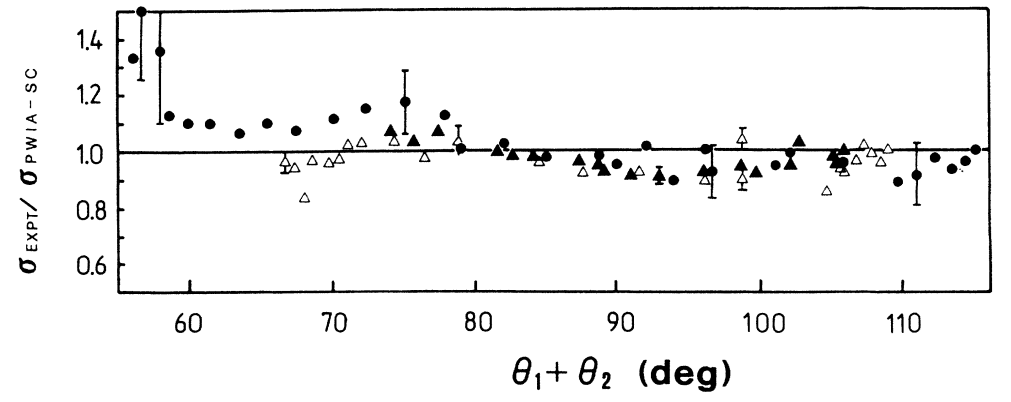

FIG. 5. The ratio $\sigma_{expt}/\sigma_{theor}$ between the measured $(e,2e)$ cross section and the theoretical value calculated in the present PWIA-SC is plotted vs the relative scattering angle $\theta_1 + \theta_2$, for coplanar asymmetric reactions where $E_1 = E_2$, $\theta_1 \neq \theta_2$, and $q \simeq \cos t = 1.0 a_0^{-1}$. The incident energy is 215 eV (●), data of Camilloni *et al.*, Ref. 33, and 406 (△) and 790 eV (▲), data of Camilloni *et al.*, Ref. 18. Each set of data has been normalized to the PWIA-SC value at the largest scattering angle.

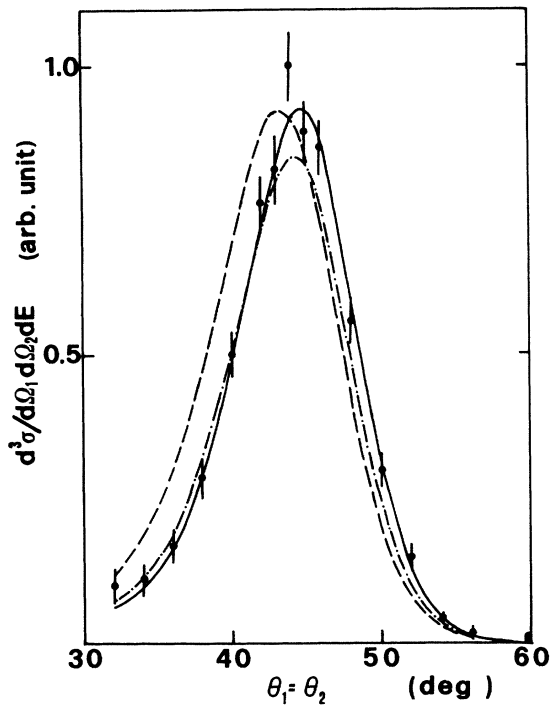

FIG. 6. The H $(e,2e)$ angular correlation measured in coplanar symmetric geometry at 413.6 eV incident energy. The relative experimental data of Weigold *et al.*, Ref. 10, are compared with PWIA (— — —), EWIA ($\bar{V}$=13 eV) (—·—·—·), and the present PWIA-SC (——) results. The experimental data have been normalized to best fit the PWIA-SC curve.

predicting the shape of the angular distributions. The asymmetric conditions confirm the accuracy of the present model everywhere but at the smaller scattering angle ($\theta_1 = 30°$).

IV. CONCLUSIONS

The pure plane-wave-impulse-approximation model has been extended to include the long-range tails of the Coulomb interaction in the final state of $(e,2e)$ processes. The basic idea for the PWIA-SC model is to subdivide the interaction space in two regions. In the inner region the collision is described by an impulsive model. In the outer region a simple semiclassical model accounts for the three-body effects due to mutual interaction of the two emerging electrons between themselves and with the ion. The parameter r_0 is the radius of the boundary sphere between the two spaces. For the sake of consistency the parameter has to be large enough to allow for the correct asymptotic behavior of the scattered wave function with respect to the short-range forces responsible for the impulsive collision. Conversely, in order to fully account for the Coulomb tails, r_0 should be as small as possible. Comparison with experiments has suggested an r_0 value close to the expectation value of the orbital radius involved in the ionization process. This value is a reasonable compromise for the above-mentioned requests, thus allowing for a straightforward application of the model whenever a valence orbital is ionized. For inner-shell ioni-

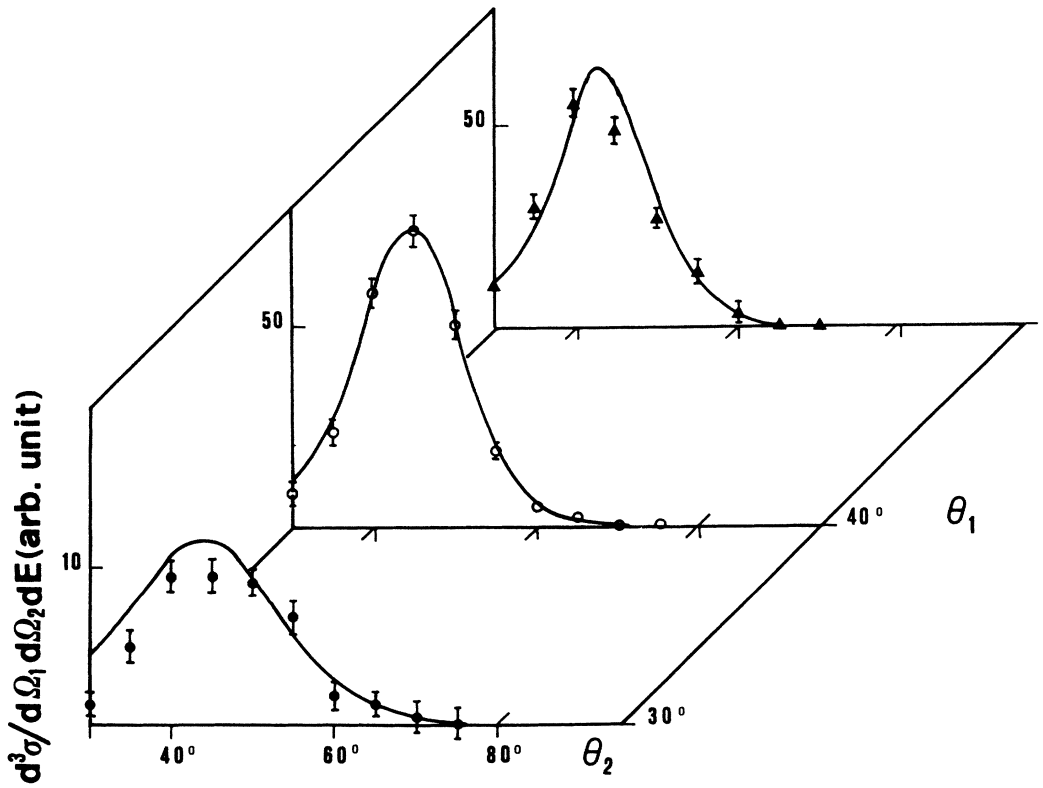

FIG. 7. The H $(e,2e)$ cross section, relative to coplanar geometry at 413.6 eV incident energy and $E_1 = E_2$, is plotted as a function of θ_1 and θ_2. The solid curve is the present PWIA-SC result. The experimental data are those of Weigold *et al.*, Ref. 10.

zation much care must be taken in applying the PWIA-SC. In this case the outer region should include the charge density of the valence orbitals, so that further interactions of the final electrons are to be taken into account in the semiclassical approximation.

This work has shown PWIA-SC to be a realistic model provided the incident energy is larger than 200 eV and the kinetic energies of the final electrons are comparable. Under these conditions, the $(e,2e)$ angular distribution shapes are very well predicted, especially concerning the smaller scattering angles. At lower incident energies and momentum transfer, when the impulsive assumptions are no more valid, the model should not be expected to work.

Anyway, the good agreement between PWIA-SC and experiments achieved in the impulsive regime suggests that the long-range e-e correlations in the final state are relevant and should be introduced for a complete description of the $(e,2e)$ reaction mechanism.

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