PHYSICAL REVIEW A VOLUME 5, NUMBER 6 JUNE 1972

Eikonal Theory of Inelastic Electron-Atom Scattering at Intermediate Energies*

Joseph C. Y. Chen
Department of Physics and Institute for Pure and Applied Physical Sciences,
University of California, San Diego, La Jolla, California 92037

and

Charles J. Joachain† and Kenneth M. Watson
Department of Physics and Lawrence Radiation Laboratory, Berkeley, California 94720

(Received 17 September 1971)

An eikonal distorted-wave theory is proposed for inelastic electron-atom collisions at intermediate energies. The primary interaction, responsible for the transition, is treated to first order, while the initial- and final-state interactions are taken into account by using the eikonal approximation. Direct and exchange collisions are both considered. Detailed numerical calculations are performed for the excitation of the $n=2$ levels of atomic hydrogen by electron impact. The results for the differential excitation cross sections are compared with those obtained in the Glauber eikonal approximation at small scattering angles.

I. INTRODUCTION

The analysis of inelastic electron-atom collisions is a problem of long-standing interest in atomic physics. Reliable approximation methods such as the close-coupling method[1] have been devised when the relative incident energy is low, so that only a few channels play an important role. On the other hand, the Born approximation has been used extensively at high energies.

In this paper we are concerned with the region of *intermediate* energies. As an improvement over the Born approximation, we propose an *eikonal distorted-wave method*, where the optical-model[2-4] formalism and the eikonal approximation[5-6] are combined.[7] At the expense of treating to first order that part of the interaction potential which is responsible for the inelastic transition, we are able to obtain reasonably simple expressions for the scattering amplitudes. These take into account explicitly the longitudinal momentum transfer, allow the explicit evaluation of exchange effects, and may be directly applied to target atoms containing many electrons.

The basic features and the approximations in volved in our method are presented in Sec. II for the general case of a binary rearrangement collision $A+B\rightarrow C+D$. In Sec. III we apply the theory to the excitation of the $2s$ and $2p$ states of atomic hydrogen by electron impact, neglecting exchange effects. These are studied in Sec. IV. Finally, we compare in Sec. V our treatment to other approaches, particularly the "many-body eikonal" method proposed by Glauber[5] in connection with high-energy hadron-nucleus scattering, and applied recently by several authors[8-13] to the elastic and inelastic scattering of electrons by atomic hydrogen and helium.

II. EIKONAL DISTORTED-WAVE METHOD

Consider a nonrelativistic collision of the type

$$A+B\rightarrow C+D\ , \tag{2.1}$$

where the particles A, B, C, and D of masses M_A, M_B, M_C, and M_D may be "elementary" or composite. We shall describe this collision in the c.m. framework. Let $\vec{R}_i$ and $\vec{k}_i$ be, respectively, the relative coordinate and the relative momentum[14] of the particles A and B in the initial channel i. The reduced mass M_i in that channel is given by

$$M_i^{-1}=M_A^{-1}+M_B^{-1}\ . \tag{2.2}$$

The channel Hamiltonian H_i is such that

$$H_i=K_i+h_i\ , \tag{2.3}$$

where K_i is the relative kinetic-energy operator given in the position representation by

$$K_i=-(1/2M_i)\nabla_{\vec{R}_i}{}^2 \tag{2.4}$$

and h_i is the internal Hamiltonian of channel i such that

$$h_i\,\psi_\alpha(\xi_i)=\epsilon_\alpha\,\psi_\alpha(\xi_i)\ . \tag{2.5}$$

Here the subscript α refers to a collection of quantum numbers, while ξ_i denotes a set of generalized coordinates (including spin variables when necessary) describing the internal structure of the systems A and B. If h_A and h_B are the internal Hamiltonians of A and B, with

$$\begin{aligned} h_A\varphi_A(s_A)&=\epsilon_A\varphi_A(s_A)\ ,\\ h_B\varphi_B(s_B)&=\epsilon_B\varphi_B(s_B)\ , \end{aligned} \tag{2.6}$$

one has

$$h_i=h_A+h_B\ ,$$

$$\epsilon_\alpha=\epsilon_A+\epsilon_B\ ,$$

$$\psi_\alpha(\xi_i) = \varphi_A(s_A)\,\varphi_B(s_B) . \qquad (2.7)$$

The total energy available in the c. m. system in channel i is

$$E_a \equiv E_{i,\alpha} = k_i^2/2M_i + \epsilon_A + \epsilon_B = k_i^2/2M_i + \epsilon_\alpha , \qquad (2.8)$$

where we have used the notation $a \equiv (i, \alpha)$. The channel eigenfunctions or asymptotic states $\chi_a \equiv \chi_{i,\alpha}$ such that

$$H_i \chi_a = E_a \chi_a \qquad (2.9)$$

are given in the coordinate representation by

$$\chi_a(\vec{r}_i, \xi_i) = (2\pi)^{-3/2} e^{i\vec{k}_i\cdot\vec{R}_i}\, \psi_\alpha(\xi_i) . \qquad (2.10)$$

Finally, if the interaction between the systems A and B is denoted by V_i, we have

$$H = H_i + V_i , \qquad (2.11)$$

where H is the total Hamiltonian of the system.

Completely similar formulas clearly hold in the final channel f with the substitutions $i \to f$, $\alpha \to \beta$, $A \to C$, and $B \to D$.

Let us now suppose that the scattering proceeds from an initial state $\chi_a \equiv \chi_{i,\alpha}$ to a final state $\chi_b \equiv \chi_{f,\beta}$. The differential cross section for this process is given by

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} M_i M_f |T_{ba}|^2 , \qquad (2.12)$$

where T_{ba} is the T matrix on the energy-momentum shell. Thus,

$$T_{ba} = \langle \chi_b | V_f | \Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)} | V_i | \chi_a \rangle , \qquad (2.13)$$

where $\Psi_a^{(+)}$ and $\Psi_b^{(-)}$ are the state vectors given by

$$\begin{aligned} \Psi_a^{(+)} &= \chi_a + (E - H + i\eta)^{-1} V_i \chi_a , \\ \Psi_b^{(-)} &= \chi_b + (E - H - i\eta)^{-1} V_f \chi_b \quad (\eta \to 0^+) . \end{aligned} \qquad (2.14)$$

Let us now suppose that the interaction potentials are decomposed in the initial and final channels as

$$\begin{aligned} V_i &= U_i + W_i , \\ V_f &= U_f + W_f . \end{aligned} \qquad (2.15)$$

We define the new Hamiltonians $\tilde{H}_i = H_i + U_i$, $\tilde{H}_f = H_f + U_f$ and assume that the corresponding state vectors

$$\begin{aligned} \phi_a^{(+)} &= \chi_a + (E - \tilde{H}_i + i\eta)^{-1} U_i \chi_a , \\ \phi_b^{(-)} &= \chi_b + (E - \tilde{H}_f - i\eta)^{-1} U_f \chi_b \end{aligned} \qquad (2.16)$$

are known. A simple calculation starting from the integral representations (2.13) of the T matrix element yields the *two potential formulas*

$$\begin{aligned} T_{ba} &= \langle \phi_b^{(-)} | V_i - W_f | \chi_a \rangle + \langle \phi_b^{(-)} | W_f | \Psi_a^{(+)} \rangle , \\ T_{ba} &= \langle \chi_b | V_f - W_i | \phi_a^{(+)} \rangle + \langle \Psi_b^{(-)} | W_i | \phi_a^{(+)} \rangle , \end{aligned} \qquad (2.17)$$

which explicitly incorporate our knowledge of $\phi_a^{(+)}$ and $\phi_b^{(-)}$ into the expression of T_{ba}.

A physically meaningful separation of V_i and V_f may be accomplished if we first choose

$$\begin{aligned} U_i &\equiv U_i(\vec{R}_i) , \\ U_f &\equiv U_f(\vec{R}_f) , \end{aligned} \qquad (2.18)$$

so that the potentials U_i and U_f only induce elastic scattering. The corresponding wave functions $\phi_a^{(+)}$ and $\phi_b^{(-)}$ are called *distorted waves* and Eqs. (2.17) become, for inelastic or rearrangement collisions,

$$T_{ba} = \langle \phi_b^{(-)} | W_f | \Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)} | W_i | \phi_a^{(+)} \rangle . \qquad (2.19)$$

The formulas (2,19) are still rigorous if the choice (2.18) of distorting potentials is made. By approximating

$$\Psi_a^{(+)} \simeq \phi_a^{(+)} , \quad \Psi_b^{(-)} \simeq \phi_b^{(-)} , \qquad (2.20)$$

and substituting into Eq. (2.19), we obtain the *distorted-wave Born approximation* (DWBA) for the transition amplitude

$$T_{ba}^{\text{DWBA}} = \langle \phi_b^{(-)} | W_i | \phi_a^{(+)} \rangle = \langle \phi_b^{(-)} | W_f | \phi_a^{(+)} \rangle . \qquad (2.21)$$

Before we proceed with Eq. (2.21), it is important to specify our choice of the potentials U_i and U_f. Any interaction which satisfies Eq. (2.18)—and therefore forbids excitation or rearrangement—clearly leads to Eq. (2.20), but the most natural choice is to adopt for U_i and U_f the *optical potentials* describing elastic scattering, respectively, in the initial and final channels. The reaction (2.1) may then be pictured as in Fig. 1, where elastic scattering in the initial (final) channel precedes (follows) a single interaction induced by W_i of W_f. The interpretation of the reaction

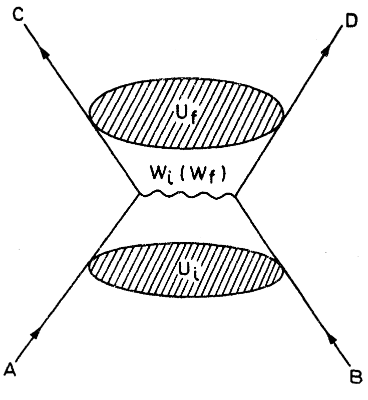

FIG. 1. Schematic representation of the primary interaction W_i (or W_f)—treated to first order—and the initial- and final-state interactions U_i and U_f—treated to all orders—in the DWBA matrix element (2.21) for a binary rearrangement collison $A + B \to C + D$.

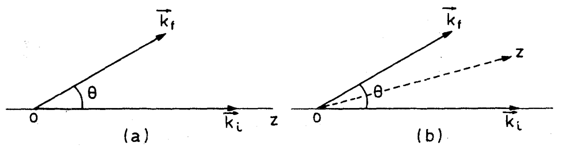

FIG. 2. Two choices of the Z axis adopted in this paper: (a) case I, Z axis along $\vec{k}_i$; (b) case II, Z axis along the bisector of the scattering angle θ.

in terms of the primary interactions W_i (W_f) and the initial- and final-state interactions U_i and U_f is then obvious.

We now return to the DWBA transition matrix element [Eq. (2.21)] and observe that when the conditions of validity of the eikonal approximation apply we may write (in the "straight-line" approximation)

$$\begin{aligned}\phi_a^{(+)} &\simeq \phi_a^{\text{eik}} = (2\pi)^{-3/2}\exp\left[i\vec{k}_i\cdot\vec{R}_i - \frac{i}{v_i}\int_{-\infty}^{Z_i} U_i(\vec{R}_i,\ Z'_i)dZ'_i\right]\psi_\alpha(\xi_i)\ ,\\ \phi_b^{(-)} &\simeq \phi_b^{\text{eik}} = (2\pi)^{-3/2}\exp\left[i\vec{k}_f\cdot\vec{R}_f - \frac{i}{v_f}\int_{\infty}^{Z_f} U_f(\vec{B}_f,\ Z'_f)dZ'_f\right]\psi_\beta(\xi_f)\ ,\end{aligned} \tag{2.22}$$

where $v_i = k_i/M_i$ and $v_f = k_f/M_f$ are the relative velocities in the initial and final channels and we have adopted a cylindrical coordinate system to decompose

$$\vec{R}_i = \vec{B}_i + Z_i\hat{Z},\quad \vec{R}_f = \vec{B}_f + Z_f\hat{Z}\ . \tag{2.23}$$

In writing Eq. (2.23), we have not yet chosen the Z axis. Two simple possibilities, illustrated on Fig. 2, will be discussed below. In case I we choose the Z axis along the incident momentum $\vec{k}_i$, while case II, corresponding to an axis chosen along the bisector of the scattering angle,[5] is somewhat closer in spirit to an evaluation of the eikonal along the classical trajectory.

The eikonal distorted-wave matrix element T_{ba}^{eik} is simply obtained by substituting the expressions (2.22) of $\phi_a^{(+)}$ and $\phi_b^{(-)}$ in Eq. (2.21). We immediately note that for direct inelastic collisions (no rearrangement), where $\vec{R}_i \equiv \vec{R}_f \equiv \vec{r}$ and $V_i = V_f = V$, we may write

$$\begin{aligned}T_{ba}^{\text{eik}} = (2\pi)^{-3}\int_0^\infty db\, b\int_{-\infty}^{+\infty} dz\\ \times\int_0^{2\pi} d\phi\exp\{i[(k_i - k_f\cos\theta)z + \delta\Phi(\vec{b}, z)]\}\\ \times\exp[-ik_f b\sin\theta\cos\phi]A(\vec{b}, z)\ .\end{aligned} \tag{2.24}$$

Here we have adopted the eikonal formulation I, so that

$$\vec{r} = \vec{b} + z\hat{k}_i\ , \tag{2.25}$$

while $(b,\ \phi)$ are the polar coordinates of b in the plane of impact parameters perpendicular to $\vec{k}_i$. Moreover,

$$\begin{aligned}\delta\Phi(\vec{b}, z) = -\frac{1}{v_i}\int_{-\infty}^{z} U_i(\vec{b}, z')dz'\\ -\frac{1}{v_f}\int_{z}^{\infty} U_f(\vec{b}, z')dz'\ ,\end{aligned} \tag{2.26}$$

and

$$A(\vec{b}, z) = \langle\psi_\beta|\,W_i\,|\,\psi_\alpha\rangle = \langle\psi_\beta|\,W_f\,|\,\psi_\alpha\rangle = \langle\psi_\beta|\,V\,|\,\psi_\alpha\rangle \tag{2.27}$$

since ψ_α and ψ_β are orthogonal and the potentials U_i and U_f only depend on $\vec{r}$.

A similar formula with slightly different kinematical factors holds for the case II. As we shall illustrate below, the integration over the azimuthal angle ϕ can often be performed, leaving a two-dimensional integral to be evaluated numerically. It is worth noting that no assumptions have been made concerning the neglect of the longitudinal momentum transfer.

For *rearrangement* collisions, where, in general, $\vec{R}_i \neq \vec{R}_f$, the eikonal distorted wave transition matrix element is clearly more difficult to evaluate. We shall return to this point in Sec. IV in connection with the exchange scattering of electrons from hydrogen atoms.

III. EXCITATION OF 2*s* AND 2*p* STATES OF HYDROGEN BY ELECTRON IMPACT

We now apply the eikonal distorted-wave method to the excitation of the 2*s* and 2*p* states of hydrogen by intermediate energy electrons, neglecting exchange effects. Let $\vec{r}$ and $\vec{r}'$ be, respectively, the coordinates of the incoming and the atomic electrons. Then we have

$$V_i = V_f = V = 1/|\vec{r} - \vec{r}'| - 1/r\ . \tag{3.1}$$

As a first approximation to the optical potentials describing the elastic scattering in the initial and final channels, we choose the corresponding static potentials. Thus, we have in the initial state

$$U_i = \langle\psi_{1s}|\,V\,|\psi_{1s}\rangle = -e^{-2r}(1/r + 1)\ , \tag{3.2}$$

while in the final states

$$U_f^{2s} = \langle \psi_{2s} | V | \psi_{2s} \rangle = -e^{-r}\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{8}\right) , \tag{3.3}$$

$$U_f^{2p0} = \langle \psi_{2p_0} | V | \psi_{2p_0} \rangle = -e^{-r}\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{24}\right) + 12 P_2(\cos\theta)\left[\frac{1}{r^3} - e^{-r}\left(\frac{1}{r^3} + \frac{1}{r^2} + \frac{1}{2r} + \frac{1}{6} + \frac{r}{24} + \frac{r^2}{144}\right)\right] , \tag{3.4}$$

$$U_f^{2p\pm1} = \langle \psi_{2p_{\pm1}} | V | \psi_{2p_{\pm1}} \rangle = -e^{-r}\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{24}\right) - 6 P_2(\cos\theta)\left[\frac{1}{r^3} - e^{-r}\left(\frac{1}{r^3} + \frac{1}{r^2} + \frac{1}{2r} + \frac{1}{6} + \frac{r}{24} + \frac{r^2}{144}\right)\right] . \tag{3.5}$$

The eikonal distorted waves (2.22) are now given by

$$\phi_a^{\text{eik}} = (2\pi)^{-3/2} \exp\left[i\vec{k}_i \cdot \vec{r} - \frac{i}{k_i}\int_{-\infty}^{z} U_i(b, z'')\, dz''\right]\psi_{1s}(r') , \tag{3.6}$$

$$\phi_b^{\text{eik}} = (2\pi)^{-3/2} \exp\left[i\vec{k}_f \cdot \vec{r} - \frac{i}{k_f}\int_{\infty}^{z} U_f^{\lambda}(b, z'')\, dz''\right]\psi_{\lambda}(r') , \tag{3.7}$$

where the index λ refers to the final states ($2s$, $2p_0$, $2p_{\pm1}$) considered here. By substituting these expressions in Eq. (2.21) and using the fact that

$$J_n(x) = (2\pi)^{-1}\int e^{ix\cos\phi}\, e^{in(\phi-\pi/2)}\, d\phi , \tag{3.8}$$

where J_n is an ordinary Bessel function of integer order n, we obtain for the various transition matrix elements (in formulation I)

$$T^{\text{eik}}_{2s,1s} = (2\pi)^{-2}\int_0^{\infty} db\, b\, J_0(k_f b \sin\theta)\int_{\infty}^{+\infty} dz\, \exp\{i[(k_i - k_f\cos\theta)z + \delta\Phi_{2s}(b, z)]\}A_{2s}(b, z) , \tag{3.9}$$

$$T^{\text{eik}}_{2p_0,1s} = (2\pi)^{-2}\int_0^{\infty} db\, b\, J_0(k_f b \sin\theta)\int_{-\infty}^{+\infty} dz\, \exp\{i[(k_i - k_f\cos\theta)z + \delta\Phi_{2p_0}(b, z)]\}A_{2p_0}(b, z) , \tag{3.10}$$

$$T^{\text{eik}}_{2p_1,1s} = (2\pi)^{-2} i\int_0^{\infty} db\, b\, J_1(k_f b \sin\theta)\int_{-\infty}^{+\infty} dz\, \exp\{i[(k_i - k_f\cos\theta)z + \delta\Phi_{2p_1}(b, z)]\}A_{2p_1}(b, z) , \tag{3.11}$$

with

$$\delta\Phi_{\lambda}(b, z) = -\frac{1}{k_i}\int_{-\infty}^{z} U_i(b, z')\, dz' - \frac{1}{k_f}\int_{z}^{\infty} U_f^{\lambda}(b, z')\, dz' \tag{3.12}$$

and

$$A_{2s}(r) = \tfrac{1}{9}\, 2^{3/2} e^{-3r/2}(r + \tfrac{2}{3}) ,$$

$$A_{2p_0}(\vec{r}) = \frac{2^{15/2}}{3^5}\,\frac{z}{r}\left[\frac{1}{r^2} - e^{-3r/2}\left(\frac{1}{r^2} + \frac{3}{2r} + \frac{9}{8} + \frac{27}{64}r\right)\right] , \tag{3.13}$$

$$A_{2p_1}(\vec{r}) = \frac{2^7}{3^5}\,\frac{b}{r}\left[\frac{1}{r^2} - e^{-3r/2}\left(\frac{1}{r^2} + \frac{3}{2r} + \frac{9}{8} + \frac{27}{64}r\right)\right] .$$

As an example we display in Fig. 3 several Argand diagrams for the $1s \rightarrow 2s$ transition at 100 eV and various values of the scattering angle. The phases of the distorted-wave amplitudes are seen to differ appreciably from the Born result. The differential cross sections for the excitation of the $2s$ state at 50, 100, and 150 eV are shown on Figs. 4–6. We note that the distortion effects reduce significantly the differential cross section in the forward direction. It is also worth looking at the differences between the two formulations of the eikonal calculation. These differences, which give a qualitative idea of the error introduced by using the "straight-line" eikonal approximation, become important at the largest angles considered here. Our results for the excitation of the $2p$ states are shown on Figs. 7–9, with the quantization axis chosen along the incident direction $\vec{k}_i$. We first note that there is no selection rule $\Delta m = \pm 1$ for s-p transitions, in contrast to the eikonal calculation of Ref. 11. We shall return to this point in Sec. V. We also see that distortion effects act in op-

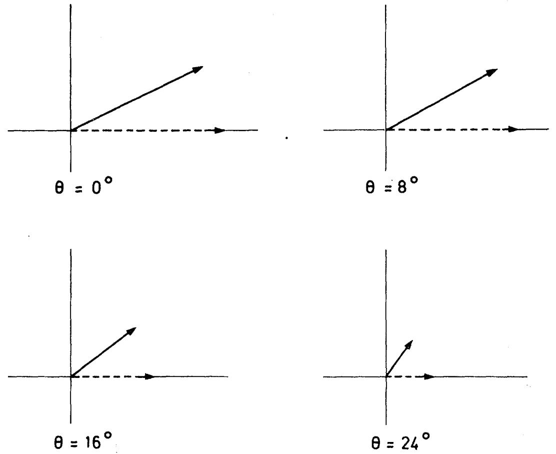

FIG. 3. Argand diagrams for the direct transition matrix element corresponding to the excitation of the $2s$ state of atomic hydrogen by electron impact at an incident electron energy $E = 100$ eV and various scattering angles. Solid arrow: eikonal DWBA (case II); dashed arrow: first Born approximation.

posite directions for the excitation of the $2p_0$ and $2p_{\pm 1}$ states, so that the net result—for the total process $1s \rightarrow 2p$—remains small. Another interesting quantity is the polarization of the radiation emitted from the $2p$ states, arising from the relative population of the excited magnetic substates. Because of the possibility of large-angle errors introduced by our use of the eikonal method, we have not attempted here to study systematically the required total cross sections, particularly at low energies. As an example, however, we find that our (energy-dependent) polarization fraction is given at 150 eV by $P = -0.03$, in closer agreement with the experimental value of Ott *et al.*[15] than the (energy-independent) result $P = -\frac{3}{11} = -0.27$ of Ref. 11.

IV. EXCHANGE EFFECTS

We now turn to the analysis of exchange effects. As an example we shall study in detail the case of the $1s \rightarrow 2s$ transition. Denoting by $T_{\text{ex}}^{\text{eik}}$ the corresponding eikonal transition matrix element, we find from Eq. (2.21) that

$$T_{\text{ex}}^{\text{eik}} = (2\pi)^{-3} \int d\vec{\text{r}}\, d\vec{\text{r}}\,' \exp\left[-i\vec{\text{k}}_f \cdot \vec{\text{r}}\,' - \frac{i}{k_f} \int_{z'}^{\infty} U_f(b', z'')\, dz'' \right] \psi_{2s}(r)$$
$$\times \left(\frac{1}{|\vec{\text{r}} - \vec{\text{r}}\,'|} - \frac{1}{r} - U_i(r) \right) \exp\left[i\vec{\text{k}}_i \cdot \vec{\text{r}} - \frac{i}{k_i} \int_{-\infty}^{z} U_i(b, z'')\, dz'' \right] \psi_{1s}(r'), \tag{4.1}$$

where U_i and U_f are given, respectively, by Eqs. (3.2) and (3.3). We have used here the "prior" form of Eq. (2.21); the "post-prior" discrepancy introduced by our use of eikonal wave functions in the initial and final channels (instead of the exact distorted waves corresponding to the potentials U_i and U_f) should be small at the angles and energies considered here.

Since the numerical evaluation of the expression (4.1) would require an unreasonable amount of computational effort, we have simplified it as follows. From the form of the potentials U_i and U_f, we note that final-state interactions are much more important than initial-state ones. This effect is easy to understand physically, since the outgoing electron moves in the field of an excited hydrogen atom in the $2s$ state, while the incoming electron feels the weaker potential produced by a hydrogen atom in the ground state. We have therefore neglected initial state interactions and written the expression (4.1) as

$$T_{\text{ex}}^{\text{eik}} \simeq (2\pi)^{-3} \int d\vec{\text{r}}\, d\vec{\text{r}}\,' \exp\left[-i\vec{\text{k}}_f \cdot \vec{\text{r}}\,' - \frac{i}{k_f} \int_{z'}^{\infty} U_f(b', z'')\, dz'' \right] \psi_{2s}(r) \left(\frac{1}{|\vec{\text{r}} - \vec{\text{r}}\,'|} - \frac{1}{r} - U_i(r) \right) e^{i\vec{\text{k}}_i \cdot \vec{\text{r}}} \psi_{1s}(r'). \tag{4.2}$$

Let us first dispose of the contribution of the two last terms in large parentheses. Since these terms do not depend on $\vec{\text{r}}\,'$, the corresponding matrix elements are easily reduced to two-dimensional integrals of the type already encountered in our study of direct collisions. The only difficulty arises from the contribution of the first term in large parentheses, which we denote by I. Writing

$$\psi_{1s}(r') = Ae^{-r'}, \qquad A = \pi^{-1/2}$$
$$\psi_{2s}(r) = B(2 - r)e^{-r/2}, \quad B = (32\pi)^{-1/2} \tag{4.3}$$

and using the fact that

$$\frac{1}{|\vec{\text{r}} - \vec{\text{r}}\,'|} = (2\pi^2)^{-1} \int d\vec{\text{K}}\, \frac{1}{K^2} e^{i\vec{\text{K}} \cdot (\vec{\text{r}}\,' - \vec{\text{r}})}, \tag{4.4}$$

we find that

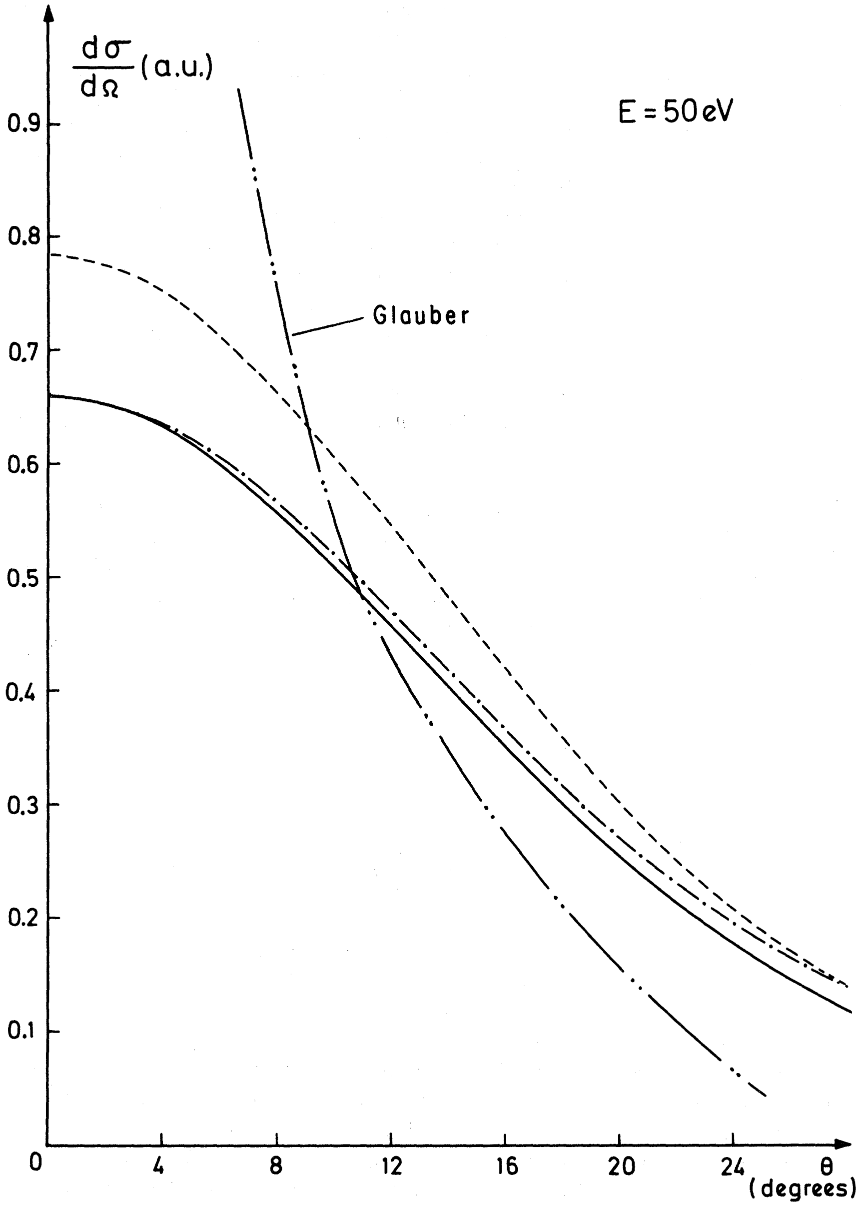

FIG. 4. Differential cross section for direct excitation of the $2s$ state of atomic hydrogen by electron impact at an incident electron energy $E = 50$ eV. Solid line: eikonal DWBA (case II); dot-dashed line: eikonal DWBA (case I); dashed line: first Born approximation; double-dot–dashed line: Glauber eikonal approximation (Ref. 11).

$$I = C\int d\vec{r}\,'\exp\left[-i\vec{k}_f\cdot\vec{r}\,' - \frac{i}{k_f}\int_{z'}^{\infty} U_f(b',z'')\,dz''\right] e^{-r} F(\vec{k}_1,\vec{r}\,'),$$

with

$$F(\vec{k}_i,\ \vec{r}\,') = \int d\vec{K}\,\frac{1}{K^2}e^{i\vec{K}\cdot\vec{r}\,'}\left[\left(\tfrac{1}{4}+|\vec{K}-\vec{k}_i|^2\right)^{-2} - \tfrac{1}{2}\left(\tfrac{1}{4}+|\vec{K}-\vec{k}_i|^2\right)^{-3}\right]. \tag{4.6}$$

and $C = \pi^{-4}AB$. Using cylindrical coordinates with the z axis along the incident momentum $\vec{k}_i$, and writing

$$\vec{K} = \vec{K}_\perp + K_z\hat{k}_i\,,\quad \vec{r}\,' = \vec{b}\,' + z'\hat{k}_i\,,$$

we have

$$F(k_i,\ b',\ z') = \int_0^\infty dK_\perp K_\perp \int_{-\infty}^{+\infty} dK_Z \int_0^{2\pi} d\alpha\,(K_\perp{}^2 + K_Z{}^2)^{-1} e^{iK_\perp b'\cos\alpha} e^{iK_z z'}$$

$$\times\left[\left(\tfrac{1}{4}+K_\perp{}^2+K_z{}^2+k_i{}^2-2K_zk_i\right)^{-2}-\tfrac{1}{2}\left(\tfrac{1}{4}+K_\perp{}^2+K_z{}^2+k_i{}^2-2K_zk_i\right)^{-3}\right], \tag{4.7}$$

where α is the angle between the vectors $\vec{K}_\perp$ and $\vec{b}'$. The integration over α is easily performed, and yields

$$F(k_i,\ b',\ z')=2\pi\left[F_1(k_i,\ b',\ z')-\tfrac{1}{2}F_2(k_i,\ b',\ z')\right], \tag{4.8}$$

with

$$F_1(k_i,\ b',\ z')=\int_0^\infty dK_\perp K_\perp J_0(K_\perp b')\int_{-\infty}^{+\infty} dK_z\,\frac{e^{iK_zz'}}{(K_\perp{}^2+K_z{}^2)(\frac{1}{4}+K_\perp{}^2+K_z{}^2+k_i{}^2-2K_zk_i)^2}, \tag{4.9}$$

$$F_2(k_i,\ b',\ z')=\int_0^\infty dK_\perp K_\perp J_0(K_\perp b')\int_{-\infty}^{+\infty} dK_z\,\frac{e^{iK_zz'}}{(K_\perp{}^2+K_z{}^2)(\frac{1}{4}+K_\perp{}^2+K_z{}^2+k_i{}^2-2K_zk_i)^3}. \tag{4.10}$$

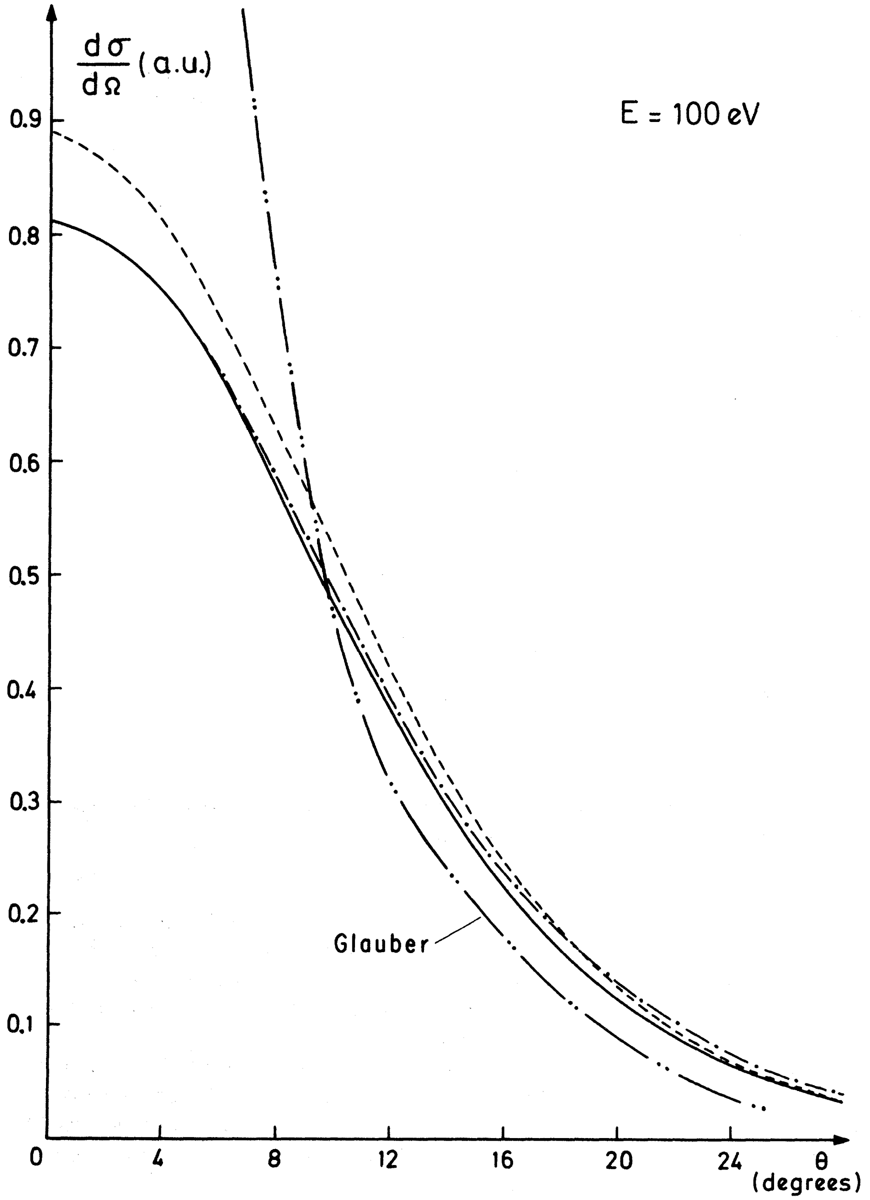

FIG. 5. Same as Fig. 4, but for $E = 100$ eV.

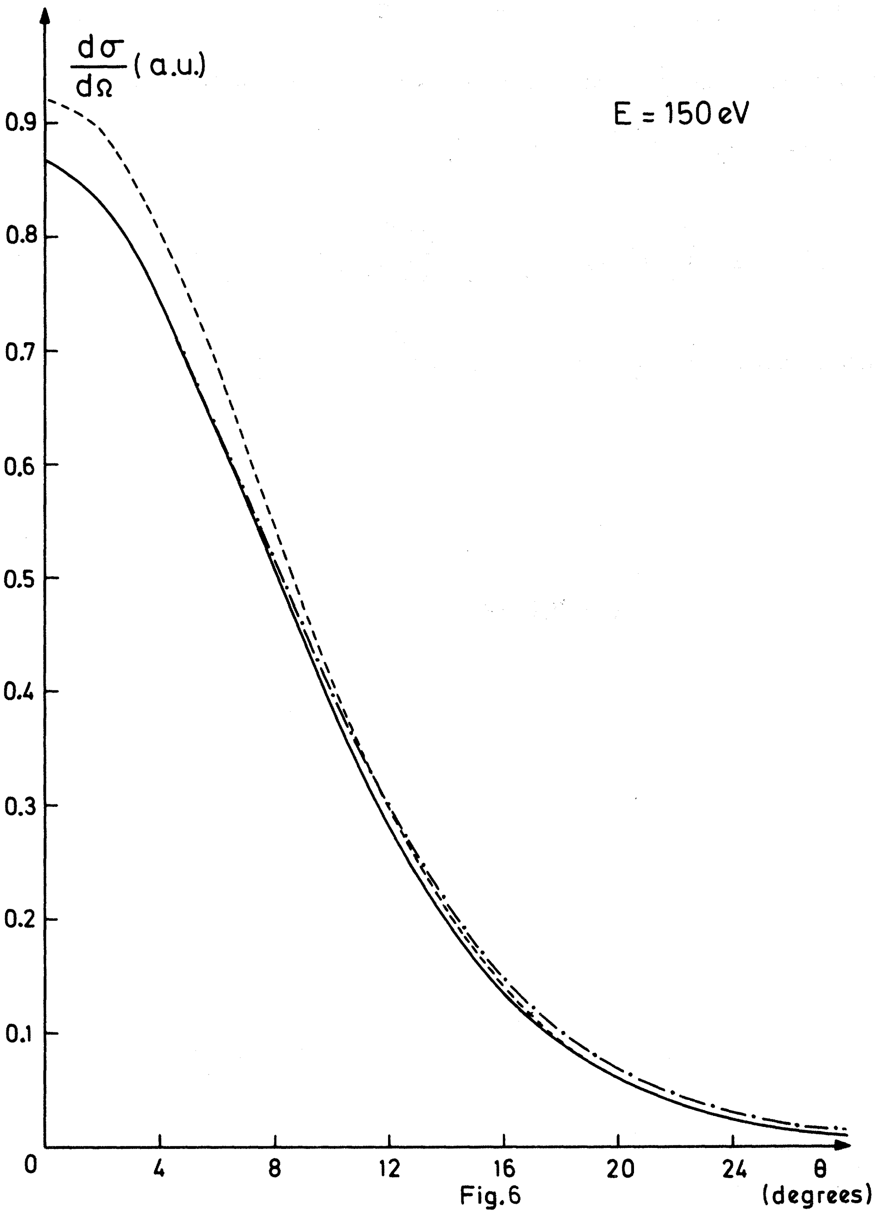

FIG. 6. Same as Fig. 4, but for $E = 150$ eV.

Finally, the quadrature over the K_z variable may be performed by contour integration in the complex K_z plane, leaving a one-dimensional integral to be performed for each value of k_i, b', and z'. By substitution of the resulting $F(k_i, b', z')$ in Eq. (4.5), we then find the contribution of the term $|\vec{r} - \vec{r}\,'|^{-1}$ to the eikonal distorted-wave matrix element (4.2).

As an example, we show in Fig. 10 the Argand diagrams corresponding to the transition matrix element (4.2) at an electron incident energy of 100 eV and for various scattering angles. As in the case of direct scattering there are significant phase differences between the distorted-wave values and the corresponding Born quantities obtained from the expression

$$T_{\text{ex}}^{\text{Born}} = \langle \chi_b | V_i \text{ (or } V_f) | \chi_a \rangle \,, \qquad (4.11)$$

by using the Feynman[16] parametrization technique and performing the last integral numerically. Moreover, we note that the magnitude of the exchange matrix element is profoundly modified near the forward direction.

The differential cross section for the excitation of the 2s state of hydrogen by electron impact, including exchange, may be written (for a random mixture of initial spin states and all final spin states)

$$\frac{d\sigma}{d\Omega}=(2\pi)^4\frac{k_f}{k_i}\left(\tfrac{1}{4}\left|T_{\rm dir}^{\rm eik}+T_{\rm ex}^{\rm eik}\right|^2+\tfrac{3}{4}\left|T_{\rm dir}^{\rm eik}-T_{\rm ex}^{\rm eik}\right|^2\right)\,, \tag{4.12}$$

where $T_{\rm dir}^{\rm eik}$ is obtained from Eq. (3.9) and $T_{\rm ex}^{\rm eik}$ is given by Eq. (4.2). Since the direct transition matrix element completely dominates the exchange one at small angles, the large difference between $T_{\rm ex}^{\rm Born}$ and $T_{\rm ex}^{\rm eik}$ near the forward direction has only little influence on the differential cross section. In fact, as we see from Figs. 11–13, distortion effects on the direct transition amplitude (i.e., of the type calculated in Sec. III) are by far the most important ones near the forward direction, even at an incident energy of 50 eV. As the scattering angle increases, exchange effects become more important until the two effects are comparable for $\theta > 20°$.

Although exchange effects are overwhelmed here by the direct transition amplitude at small angles, it is worth insisting on the fact that distortion effects significantly modify the exchange transition amplitude near the forward direction. Such effects could be responsible for important departures from the Born approximation when the direct term is *not* present. This is the case, for example, in the excitation of triplet states of helium by electron impact, in particular the 2^3S state, where experi-

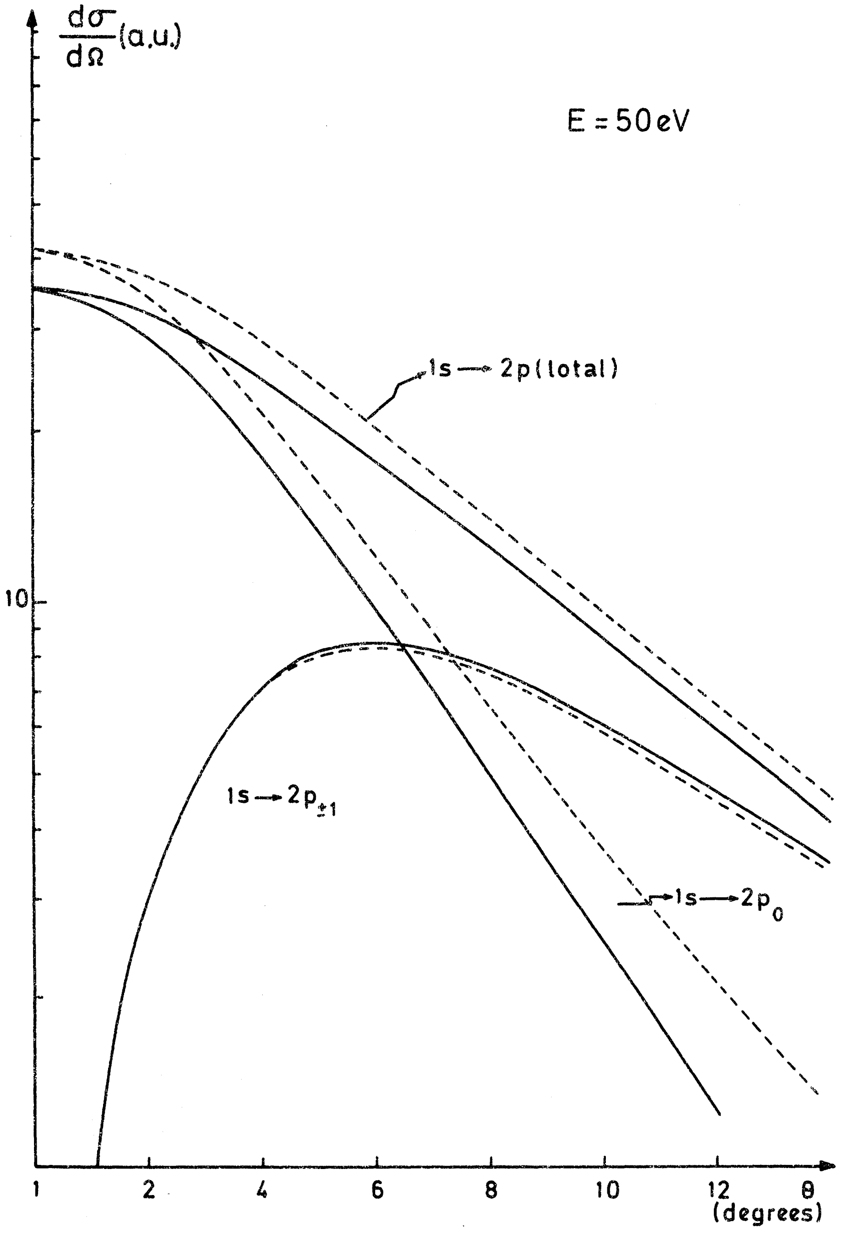

FIG. 7. Differential cross section for direct excitation of the $2p$ states of atomic hydrogen by electron impact at an incident electron energy $E = 50$ eV. Solid line: eikonal DWBA (case I); dashed line: first Born approximation.

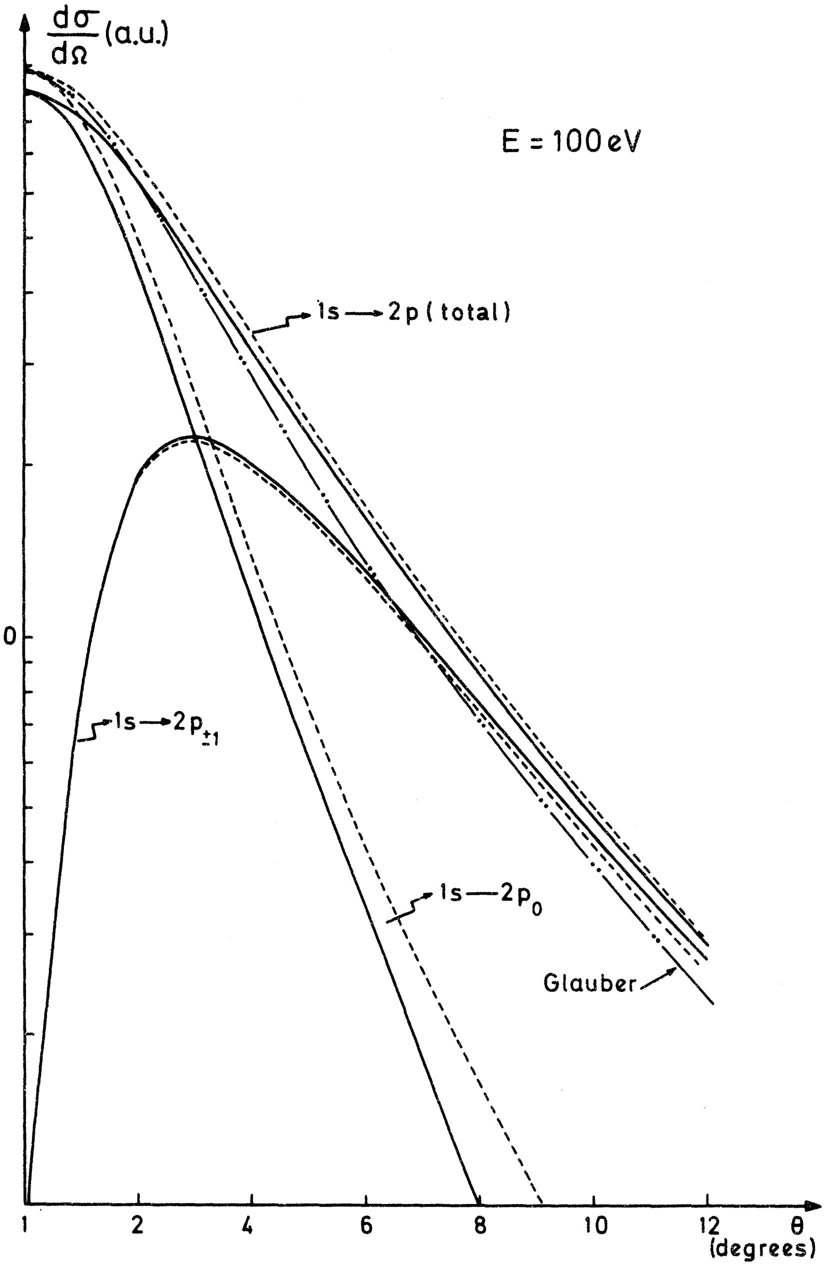

FIG. 8. Same as Fig. 7., but for $E = 100$ eV. The double-dot—dashed line is the Glauber eikonal approximation (Ref. 11).

ments[17,18] performed at intermediate energies and small angles disagree strongly with the Born predictions. A recent calculation[13] using the "many-body" eikonal approximation (to be discussed in Sec. V) lends strong support to this point of view.

V. DISCUSSION

We begin by comparing our work with the Glauber eikonal approximation which has recently been applied extensively to electron-atom scattering. This method is based on the following ansatz for the total state vector:

$$\psi_a^{(+)} \simeq (2\pi)^{-3/2} \exp\left[i\vec{k}_i \cdot \vec{R}_i - \frac{i}{v_i}\int_{-\infty}^{Z_i} V_i(\vec{R}_i, \xi_i)\,dZ_i'\right]\psi_\alpha(\xi_i), \tag{5.1}$$

where V_i is the full interaction between the projectile and the target. The transition matrix element (2.13) is then in general a complicated multidimensional integral, whose reduction to a tractable form is difficult, even for the simplest cases. The elastic scattering of electrons by hydrogen[8,10] and helium[9] atoms has been analyzed in this way, neglecting exchange effects. The results are in good agreement with experimental data, but there is a

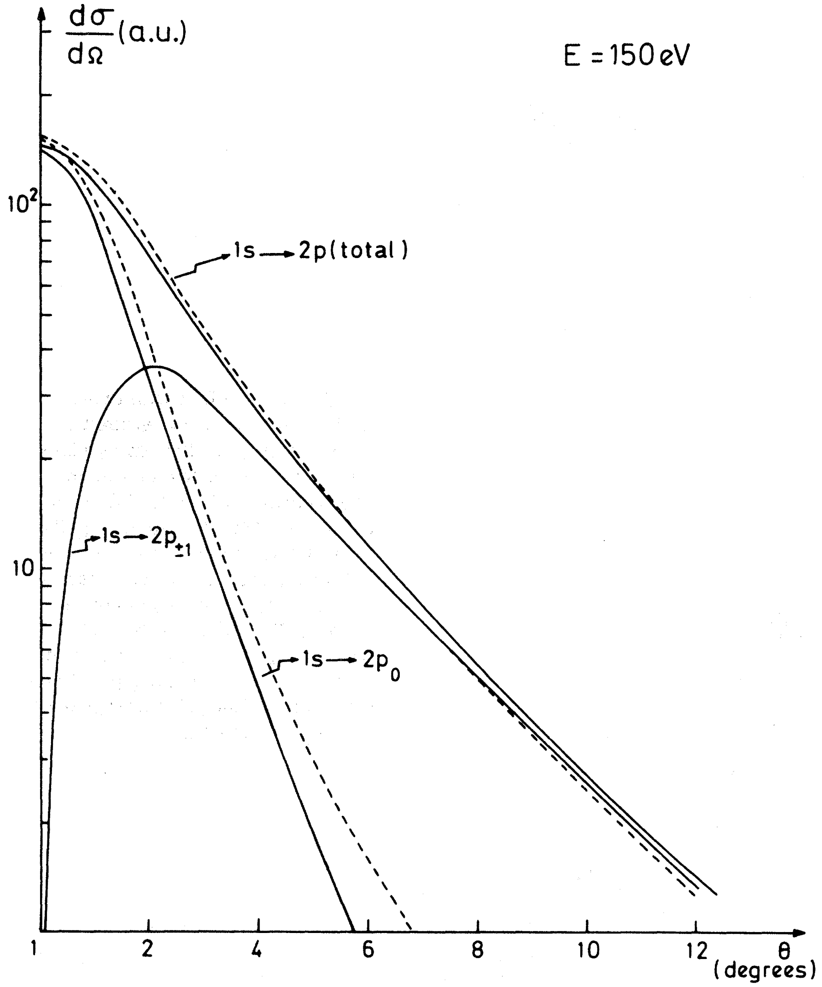

FIG. 9. Same as Fig. 7, but for $E = 150$ eV.

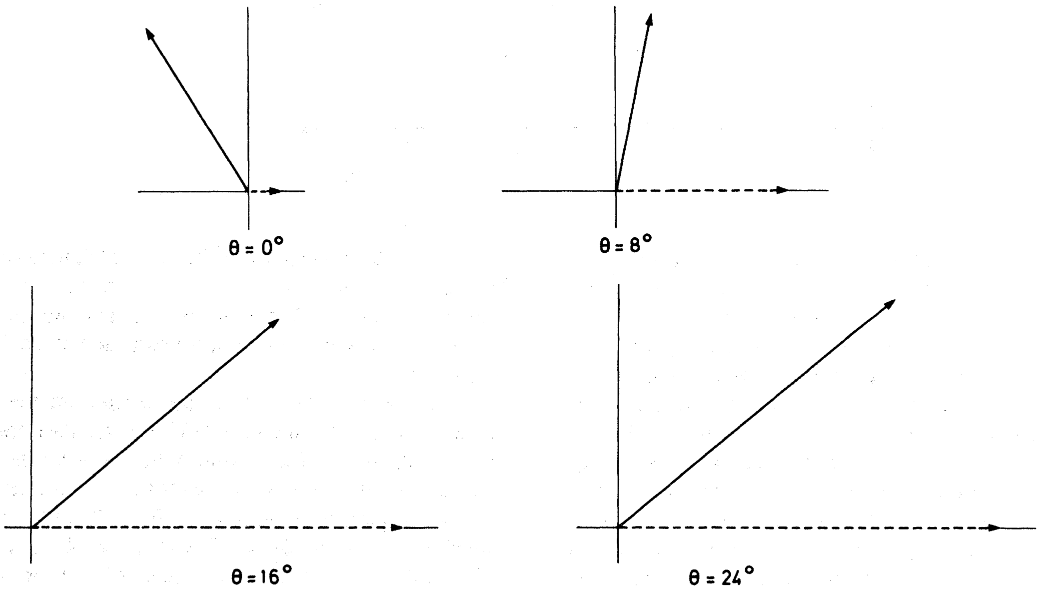

FIG. 10. Argand diagrams for the exchange transition matrix element corresponding to the excitation of the 2*s* state of atomic hydrogen by electron impact at an incident electron energy $E = 100$ eV and various scattering angles. Solid arrow: eikonal DWBA; dashed arrow: first Born approximation.

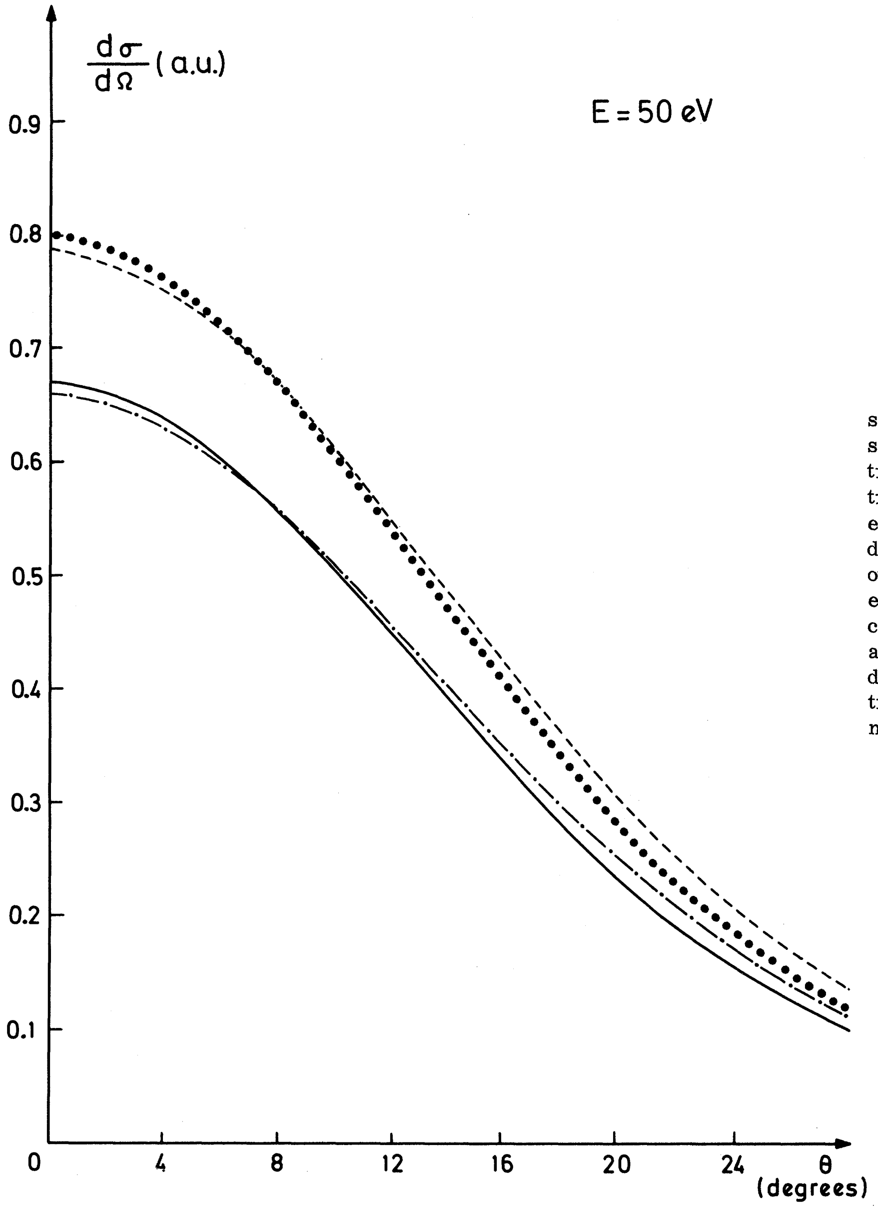

FIG. 11. Differential cross section for excitation of the $2s$ state of atomic hydrogen by electron impact at an incident electron energy $E = 50$ eV. Solid line: eikonal DWBA with exchange; dot-dashed line: eikonal DWBA without exchange. The direct matrix elements are those evaluated in case II. Dashed line: first Born approximation (without exchange); dotted line: first Born approximation with exchange (Born-Oppenheimer approximation).

serious difficulty at small angles, where the transition amplitude diverges logarithmically as the momentum transfer tends to zero.

Inelastic electron-hydrogen scattering has recently been studied using the Glauber method by Tai *et al.*[11] and Byron.[12] In order to simplify the matrix element (2.13), the first authors make the assumption that the momentum transfer is orthogonal to the incident momentum $\vec{k}_i$. For inelastic scattering, this assumption is not reasonable for both small and large scattering angles. This leads for example to the selection rule $\Delta m = \pm 1$ for $s \rightarrow p$ transitions and hence to an energy-independent polarization fraction $P = -\frac{3}{11}$ of the light emitted after the excitation of the $2p$ level. In addition, Tai *et al.* neglect exchange effects and find that the Glauber method improves on the first Born approximation at rather low energies and large angles, where the eikonal approximation is not on firm grounds.

The work of Byron[12] is also based on the Glauber eikonal approximation but does not make use of the assumption that the momentum transfer is perpendicular to the incident momentum. The multidimensional integrals appearing in Eq. (2.13) are then performed by the Monte Carlo method. The results obtained by this procedure are very encouraging, particularly with respect to the total cross sections and the polarization fraction of the light emitted in the $2p \rightarrow 1s$ transition. Although no angular distributions for the excitation of atomic hydrogen are given in Ref. 12, the total cross sections obtained are in qualitative agreement with those which we find by integrating our angular distributions. Similarly, our values of the polarization fraction are in much better agreement with those of Byron than those of Tai *et al.* Finally, we have also performed calculations for *positron* scattering which at small angles yield smaller intensities than for the corresponding electron case. These results are again in agreement with the calculations of Ref. 12 but disagree with the predictions of Ref. 11, which are the same for electrons and positrons.

Although the application of Monte Carlo techniques to evaluate the multidimensional integrals appearing in the Glauber method has been very successful in dealing with simple target atoms as hydrogen and helium,[12,13] it seems difficult to extend this technique to more complex targets. This is not the case with the eikonal distorted-wave method presented in this paper. Indeed, since the optical potentials U_i and U_f which are "eikonalized" depend only on the relative coordinates $\vec{R}_i$ and $\vec{R}_f$, the reduction of the direct and exchange scattering amplitudes proceeds for *any* atom as in the case of hydrogen. Recent calculations[19] have been done along this line for the excitation of various states of helium by electron impact, and the results are in good agreement with the absolute measurements of Chamberlain *et al.*[18]

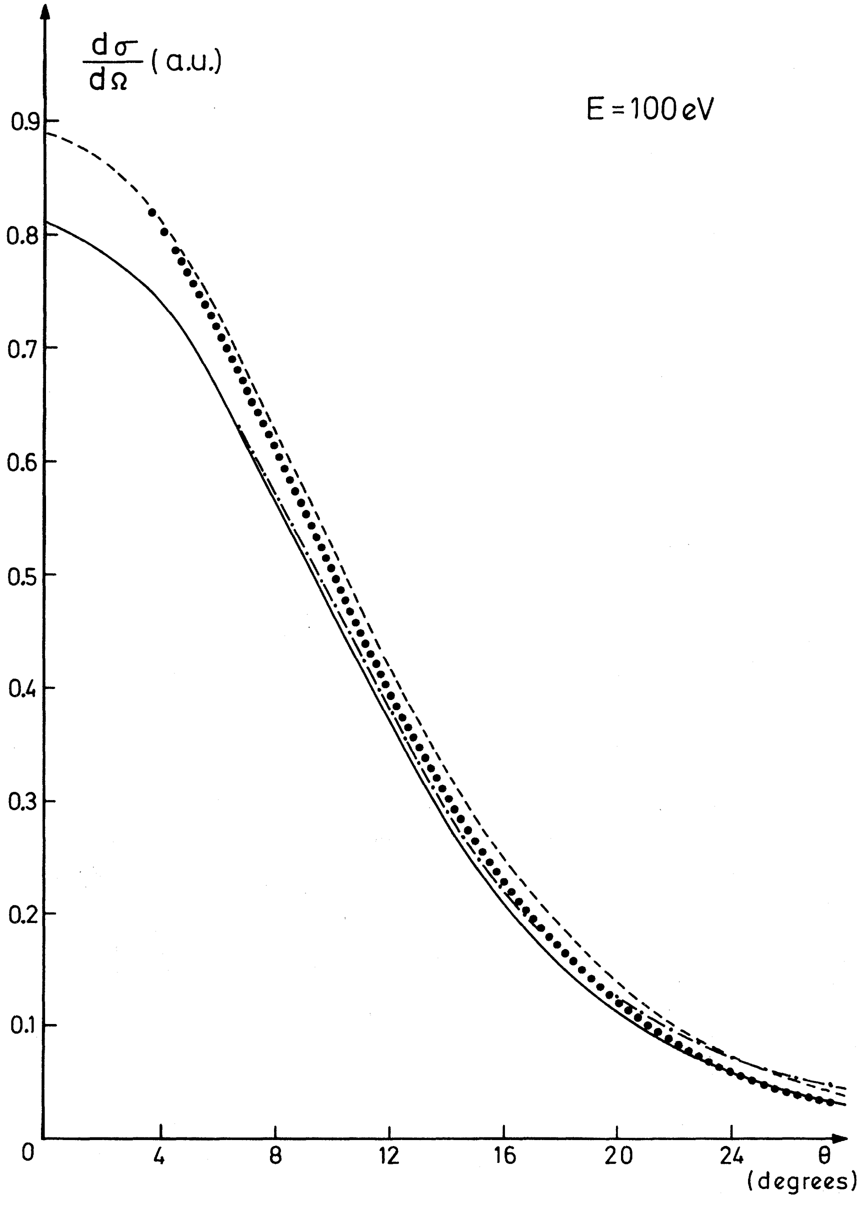

FIG. 12. Same as Fig. 11, but for $E = 100$ eV.

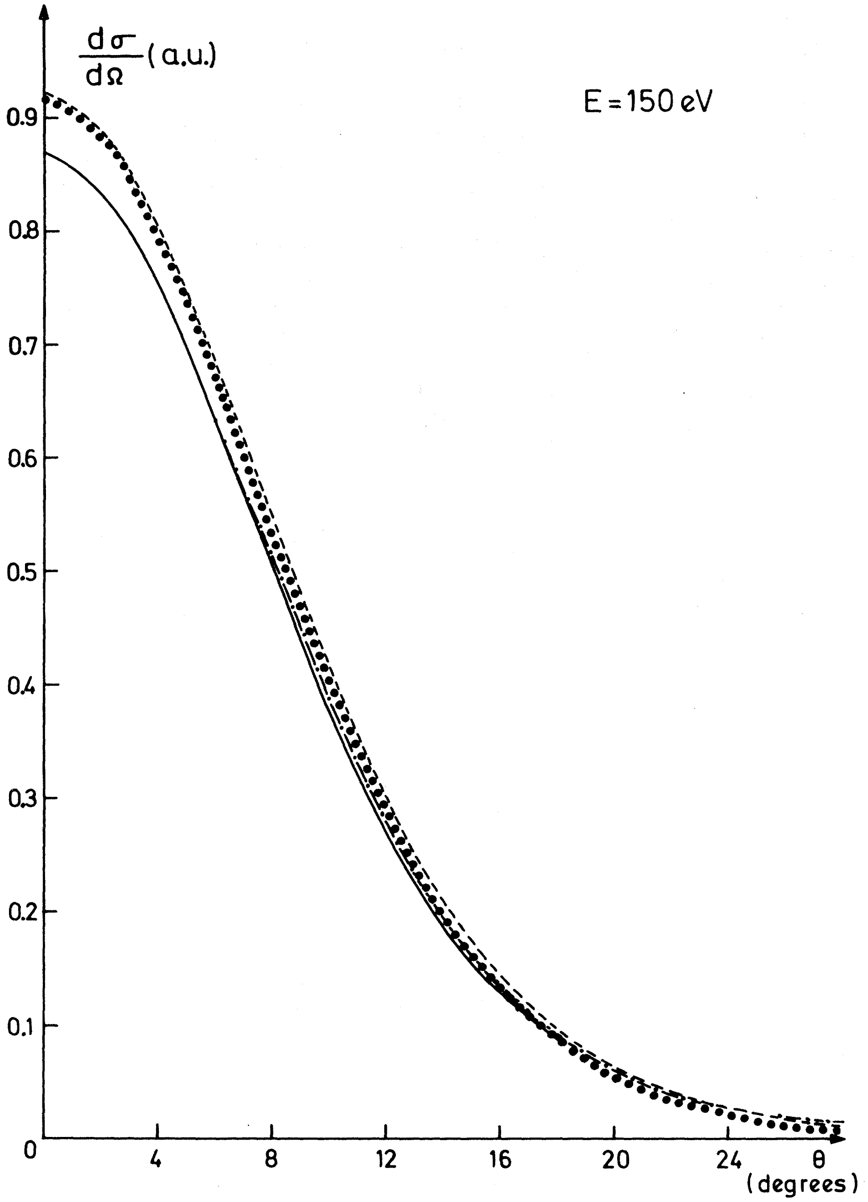

FIG. 13. Same as Fig. 11, but for $E = 150$ eV.

An obvious improvement over the method reported here would be to use the true optical potentials—describing the elastic scattering in the initial and final states—as a choice for U_i and U_f, instead of the static potentials chosen here. Such an approach has recently been proposed[20] to analyze elastic electron-helium collisions at intermediate energies, where absorption effects were found to be important. However, there are some difficulties in extending this method to inelastic collisions, since the parametrization of the absorptive part and of the long range behavior of the optical potential may be tedious, particularly in the final channel where the target is left in an excited state. It is for this reason that we have chosen here for U_i and U_f the static potentials which contain no adjustable parameters.

ACKNOWLEDGMENTS

One of us (C. J. J.) would like to thank Professor G. H. Trilling and Professor G. F. Chew for their hospitality at the Physics Department of the University of California at Berkeley and at the Lawrence Radiation Laboratory. We would like to thank the staff of the LRL Computer Center for their generous assistance. Special thanks are due Miss L. Wong for her help in solving various numerical problems connected with this work.

[*] Research supported in part by the National Science Foundation under Grant No. GP-20459; by the Atomic Energy Commission under Contract No. AT(04-3)-34, PA 196; and by the Air Force Office of Scientific Research, Office of Aerospace Research, U. S. Air Force, under Grant No. F44620-C-70-0028.

[†] Present address: Physique Théorique et Mathématique, Faculté des Sciences, Université Libre de Bruxelles, Brussels, Belgium.

[1] See, for example, N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford U. P., New York, 1965), Chap. 17.

[2] M. H. Mittleman and K. M. Watson, Phys. Rev. 113, 198 (1959); Ann. Phys. (N. Y.) 10, 268 (1960).

[3] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964), Chap. 15.

[4] A. L. Fetter and K. M. Watson, *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic, New York, 1965), Vol. 1, p. 115.

[5] R. J. Glauber, *Lectures in Theoretical Physics*, edited by W. E. Brittin (Interscience, New York, 1959), Vol. I, p. 315.

[6] J. C. Y. Chen and K. M. Watson, Phys. Rev. 188, 236 (1969).

[7] A. S. Goldhaber and C. J. Joachain [Phys. Rev. 171, 1566 (1968)] have used a similar approach to analyze production reactions in high-energy hadron-nucleus collisions.

[8] V. Franco, Phys. Rev. Letters 20, 709 (1969).

[9] V. Franco, Phys. Rev. A 1, 1705 (1970).

[10] H. Tai, P. J. Teubner, and R. H. Bassel, Phys. Rev. Letters 22, 1415 (1969); 23, 453(E) (1969).

[11] H. Tai, R. H. Bassel, E. Gerjuoy, and V. Franco, Phys. Rev. A 1, 1819 (1970).

[12] F. W. Byron, Jr., Phys. Rev. A 4, 1907 (1971).

[13] F. W. Byron, Jr. and C. J. Joachain, Bull. Am. Phys. Soc. 16, 585 (1971); Phys. Letters 38A, 185 (1972).

[14] We shall use atomic units (a.u.) throughout this paper.

[15] W. R. Ott, W. E. Kauppila, and W. L. Fite, Phys. Rev. Letters 19, 1361 (1967).

[16] R. P. Feynman, Phys. Rev. 76, 769 (1949).

[17] L. Vriens, J. A. Simpson, and S. R. Mielczarek, Phys. Rev. 165, 7 (1968).

[18] G. E. Chamberlain, J. R. Mielczarek, and C. E. Kuyatt, Phys. Rev. A 2, 1905 (1970).

[19] C. J. Joachain and R. Vanderpoorten, in *Seventh International Conference on the Physics of Electronic and Atomic Collisions* (North-Holland, Amsterdam, 1971).

[20] C. J. Joachain and M. H. Mittleman, Phys. Letters 36A, 209 (1971); Phys. Rev. A 4, 1492 (1971).

PHYSICAL REVIEW A VOLUME 5, NUMBER 6 JUNE 1972

Multiple-Scattering Effects in High-Energy Electron-Molecule Collisions. I. Diatomic Molecules

A. C. Yates and A. Tenney
Department of Chemistry, Indiana University, Bloomington, Indiana 47401

(Received 29 July 1971)

The multiple-scattering theory of Glauber is used to investigate the importance of double scattering in the collisions of fast electrons with diatomic molecules. By representing the atomic potentials as a sum of Yukawa terms, comparisons of scattering amplitudes calculated by the partial-wave analysis and the high-energy approximation (Moliere) are made over a wide range for several atoms. At 40 keV the amplitudes are found to be numerically equivalent to within a few percent, with the agreement worsening with decreasing energy. Calculations for N_2 at 0.5 and 40 keV and for I_2 and U_2 for 40-keV incident electron energies are presented; these results can be regarded as quantitative estimates of the importance of double scattering for a system of two atoms as a function of atomic number. Our U_2 calculation is compared with a similar calculation by Hoerni. In contrast to his findings, the double-scattering contribution to the differential cross section is seen to be negative in the small-angle region. In any event, for all cases considered, the multiple-scattering correction is quite small, amounting to no more than ±2% of the differential cross section for any angle of scattering.

I. INTRODUCTION

It has been suspected for some time now, that intramolecular multiple scattering may have a marked influence on the results of the electron-diffraction analysis of polyatomic molecules having two or more heavy atoms in close proximity. In fact, recent experiments by Jacob and Bartell[1] and others have suggested that the reliability of molecular parameters determined by such analyses is questionable. In addition to this a number of other experimental investigations in the medium to high-energy-electron range have indicated that the neglect of multiple scattering in theoretical models is perhaps an important source of error.[2, 3]

For the energy range being considered here (~0.5–40 keV), the usual approach to the determination of theoretical molecular intensities is to assume that incident electrons do not undergo more than one scattering within the molecule,[4] and that the effect of chemical bonding on the scattering can be neglected. The first detailed calculation of