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Eikonal optical-model theory of elastic electron-atom scattering*

F. W. Byron, Jr.†
Department of Physics, University of Massachusetts, Amherst, Massachusetts 01002

Charles J. Joachain
Physique Théorique et Mathématique, Faculté des Sciences, Université Libre de Bruxelles, Bruxelles, Belgium, and Institut de Physique Corpusculaire, Université de Louvain, Louvain-la-Neuve, Belgium

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We analyze elastic electron-atom scattering at intermediate and high energies by using a second-order optical-model potential together with the eikonal approximation. We devote particular attention to the role of long-range forces and formulate the theory in a way suitable for generalizations to complex target atoms. We also study the relationship between the optical eikonal model and the Born series, and include exchange effects to leading order in the inverse power of the energy. Our optical-model theory is then illustrated by a detailed analysis of elastic electron-helium scattering for incident-electron energies ranging from 100 to 500 eV. We find excellent agreement with experimental data without using any phenomenological parameter.

I. INTRODUCTION

Optical-model calculations of electron-atom elastic scattering have attracted considerable interest in the past few years.[1–10] Although earlier applications mostly dealt with low-energy scattering, the case of intermediate- and high-energy collisions has also been considered recently.[8–10] In this paper we shall be concerned precisely with this energy region, which we shall analyze by means of an eikonal[11] version of the optical-model formalism. Our aim is twofold. First, we want to formulate the optical eikonal model[9,10] in a form suitable for application to scattering by complex atoms, using a minimum number of phenomenological parameters. Second, we want to pursue our investigations[12–14] of the connection between eikonal methods and the Born series. In particular, we wish to elucidate the relationships between the optical eikonal model and the eikonal–Born-series (EBS) approach which we recently proposed.[14] This will be done below for the case of electron-helium scattering, where all the calculations can be performed from first principles and absolute measurements of differential cross sections are available.[15–18]

We begin in Sec. II by recalling the basic equations of the optical eikonal model.[10] After discussing briefly the static and absorption contributions to the eikonal phase, we analyze in detail the role of the long-range part of the interaction. The corresponding polarization-phase-shift function is written down for an arbitrary atom in terms of an average excitation energy (already used for the absorption part) and other known quantities. Hence the generalization of the model to complex target atoms is made by using only *one* phenomenological parameter. Moreover, an important deficiency of the eikonal method, analyzed in our previous work,[13,14] is remedied by using second-order perturbation theory. Exchange effects are also considered.

Section III is devoted to the applications of our method to the case of elastic electron-helium scattering at incident-electron energies ranging between 100 and 500 eV. In this case the average excitation energy Δ may be determined *a priori* by using accurate sum rules for the first-Born-approximation total cross section,[19] so that our optical-eikonal–model calculations do not contain any phenomenological parameter. Our results are in excellent agreement with the recent experimental data at small angles. We also compare our calculations with those which we have performed recently by using the EBS method.[14] Furthermore, we discuss higher-order terms and analyze the situation at larger angles, where the static potential dominates the scattering.[20] Finally, we compare our results for the real part of the scattering amplitude in the forward direction with calculations based on dispersion relations[21] and with the values given by our EBS method.[14]

II. OPTICAL-MODEL THEORY

A. Basic equations

Let us consider the nonrelativistic elastic scattering of an electron by a neutral atom having Z electrons. We assume that the center of mass of the atom coincides with its nucleus and choose it as the origin of our coordinate system. We label by $\vec{r}$ and $\vec{r}_i$, respectively ($i=1, 2, \ldots, Z$), the positions of the incident and atomic electrons and we shall also use the symbol X to denote all the target coordinates including (if necessary) spin variables. Since we are concerned with the scattering of fast electrons (i.e., the region of intermediate and high energies), we shall first neglect exchange effects between the incident electron and the electrons initially bound in the target. Exchange effects will be taken into account separately below by using perturbation theory. The initial and final wave vectors of the electron will be denoted by $\vec{k}_i$ and $\vec{k}_f$, respectively, with $k=|\vec{k}_i| = |\vec{k}_f|$. All quantities will be expressed in atomic units.[22]

The notation which we adopt is that of II.[14] Thus we denote the kinetic-energy operator of the projectile by $K=-\frac{1}{2}\nabla^2_{\vec{r}}$, while h is the internal target Hamiltonian with eigenkets $|n\rangle$ and eigenenergies w_n (we use the symbols $|0\rangle$ and w_0 for the ground state). The full interaction V between the projectile and the target is given by

$$V(\vec{r},X)=\sum_{i=1}^{Z}\frac{1}{|\vec{r}_i-\vec{r}|}-\frac{Z}{r}\ . \qquad (2.1)$$

We will also make use of the Born series for the direct part f_d of the scattering amplitude. That is,

$$f_d=\sum_{n=1}^{\infty}\bar{f}_{Bn}\,, \qquad (2.2)$$

where $\bar{f}_{Bn}$ is the term of the Born series which is of order n in the interaction potential V [see Eq. (2.12) of II].

We begin by writing the equivalent one-body Schrödinger equation for elastic scattering, namely,

$$(K+\mathcal{V}_{\text{opt}}-\tfrac{1}{2}k^2)\psi_i^{(+)}=0\ , \qquad (2.3)$$

where $\psi_i^{(+)}$ is the elastic-scattering wave function describing the motion of the projectile in the optical potential $\mathcal{V}_{\text{opt}}$. Neglecting for the moment exchange effects between the incident and target electrons, we may write the optical potential $\mathcal{V}_{\text{opt}}$ to second order in a multiple scattering expansion (in terms of the interaction V) as

$$\mathcal{V}_{\text{opt}}=V^{(1)}+V^{(2)}\ , \qquad (2.4)$$

where the first order or static potential is such that

$$V^{(1)}=\langle 0|V|0\rangle\ , \qquad (2.5)$$

while the second-order part $V^{(2)}$ is given by

$$V^{(2)}=\sum_{n\neq 0}\frac{\langle 0|V|n\rangle\langle n|V|0\rangle}{\frac{1}{2}k^2-K-(w_n-w_0)+i\epsilon}\,,\quad \epsilon\to 0^+\ . \qquad (2.6)$$

Here the summation runs over all the intermediate states of the target, the ground state being excluded.

The static potential $V^{(1)}$ may be readily evaluated for simple atoms, or when an independent-particle model such as the Hartree-Fock method is used to describe the ground state $|0\rangle$ of the target. We recall that since this potential is real and of short range it does not take into account absorption or polarization effects which play an important role at intermediate and high energies. However, we have shown recently[20] in a study of the elastic scattering of fast electrons by helium that intermediate- and large-angle collisions are dominated by the static potential $V^{(1)}$.

We now examine the second-order potential $V^{(2)}$. Since we are dealing with the region of intermediate and high energies we shall follow the method of Joachain and Mittleman[9,10] and replace the differences w_n-w_0 in Eq. (2.6) by an average excitation energy Δ. The sum on n which appears on the right-hand side of Eq. (2.6) can then be done by closure. Using the coordinate representation, we obtain for $V^{(2)}$ the nonlocal complex expression[10]

$$\langle\vec{r}|V^{(2)}|\vec{r}'\rangle=G_0^{(+)}(k',\vec{r},\vec{r}')A(\vec{r},\vec{r}')\ , \qquad (2.7)$$

where $G_0^{(+)}(k',\vec{r},\vec{r}')$ is the free single-particle Green's function, with $k'^2=k^2-2\Delta$ and

$$A(\vec{r},\vec{r}')=\langle 0|V(\vec{r},X)V(\vec{r}',X)|0\rangle - \langle 0|V(\vec{r},X)|0\rangle\langle 0|V(\vec{r}',X)|0\rangle\ . \qquad (2.8)$$

The resulting Schrödinger equation, obtained by substituting the above expressions in Eq. (2.3), then reads

$$[-\tfrac{1}{2}\nabla^2_{\vec{r}}+V^{(1)}(\vec{r})-\tfrac{1}{2}k^2]\psi_i^{(+)}(\vec{r}) + \int G_0^{(+)}(k',\vec{r},\vec{r}')A(\vec{r},\vec{r}')\psi_i^{(+)}(\vec{r}')\,d\vec{r}'=0\ . \qquad (2.9)$$

B. Optical eikonal theory

The above equation is still very complicated because of the structure of $A(\vec{r},\vec{r}')$. Since, as we have already mentioned, the static potential governs intermediate- and large-angle collisions, we shall only be interested in solving this equation for small-angle scattering, where absorption and polarization effects are the most important. Therefore, following the work of Joachain and Mittleman,[10] we solve Eq. (2.9) in the eikonal approximation to write the optical eikonal elastic-scattering amplitude in the form

$$f_{\rm OE} = \frac{k}{2\pi i} \int d^2 \vec{b} e^{i\vec{K}\cdot\vec{b}} (e^{i\chi_{\rm opt}(\vec{b})} - 1) , \qquad (2.10)$$

where $\vec{K} = \vec{k}_i - \vec{k}_f$ is the momentum transfer and the optical eikonal phase is given by[10,22]

$$\chi_{\rm opt}(\vec{b}) = -\frac{1}{k} \int_{-\infty}^{+\infty} V^{(1)}(\vec{b}, z)\, dz + \frac{i}{kk'} \times \int_{-\infty}^{+\infty} dz \int_{-\infty}^{z} e^{-i\xi(z-z')} A(\vec{b}, z; \vec{b}z') , \qquad (2.11)$$

with $\xi = k - k' \simeq \Delta/k$. We shall also use below the *optical Born* scattering amplitude

$$f_{\rm OB} = \frac{k}{2\pi} \int d^2\vec{b}\, e^{i\vec{K}\cdot\vec{b}} \chi_{\rm opt}(\vec{b}) , \qquad (2.12)$$

obtained by expanding the bracket in Eq. (2.10) and keeping the term linear in $\chi_{\rm opt}$.

The first term in Eq. (2.11) is simply the result one would expect from potential scattering eikonal studies, namely, the average charge-cloud potential which will be iterated to all orders of perturbation theory via Eq. (2.10). We will write this term as

$$\chi_{\rm st}(\vec{b}) = -\frac{1}{k} \int_{-\infty}^{\infty} V^{(1)}(\vec{b}, z)\, dz . \qquad (2.13)$$

The second term is more interesting; it is of order $1/k$ relative to the term in $V^{(1)}$ and has both a real and an imaginary part. The imaginary part represents the leading contribution due to open channels. We will write this term as

$$\chi_{\rm abs}(\vec{b}) = \frac{i}{kk'} \int_{-\infty}^{\infty} dz \int_{-\infty}^{z} dz' \cos\xi(z - z') A(\vec{b}, z; \vec{b}, z')$$

$$= \frac{i}{2kk'} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz'\, e^{-i\xi(z-z')} A(\vec{b}, z; \vec{b}, z') , \qquad (2.14)$$

where the fact that A is real symmetric has been used. Employing methods discussed in Ref. 10, this multiple integral (recall that a multidimensional integration is concealed in A) can be reduced to a single integral for any case in which the wave function of the target ground state can be represented as a sum of products of single-particle orbitals.

We expect the contribution of $\chi_{\rm abs}(\vec{b})$ to be most important at small angles where the amplitudes for transitions into optically allowed channels are very large. At wider angles, the optically allowed amplitudes diminish rapidly, as do all other amplitudes except the elastic amplitude; thus we expect $\chi_{\rm st}$, which represents the effect of the ground state, to dominate in all orders of perturbation theory at large angles.

Now let us look at the real part of the second term in Eq. (2.11), which we write as

$$\chi_{\rm pol}(\vec{b}) = \frac{1}{kk'} \int_{-\infty}^{\infty} dz \int_{-\infty}^{z} dz' \times \sin\xi(z - z') A(\vec{b}, z; \vec{b}, z') . \qquad (2.15)$$

It might be thought that as k becomes large (so that ξ is small) $\chi_{\rm pol}$ will become of order $1/k^2$ relative to $\chi_{\rm st}$ and hence contribute corrections or order $1/k^2$ to the first Born approximation. This, however, is not the case since if one expands the factor $\sin\xi(z - z')$ the resulting integrals for the scattering amplitude are divergent. To see what is happening in this case, it is instructive to look at the contribution of $\chi_{\rm pol}$ to the optical Born amplitude of Eq. (2.12). The quantity $\chi_{\rm pol}$ is in general very complicated, but if we are interested in the small-momentum-transfer behavior of $f_{\rm OB}$ we need primarily the large-$\vec{b}$ behavior of $A(\vec{b}, z; \vec{b}, z')$. This is readily done by expanding the potentials in Eq. (2.8) and keeping only the leading powers in $1/r$ and $1/r'$. A simple calculation gives

$$A(\vec{b}, z; \vec{b}, z') \simeq 4 \frac{zz' + b^2}{(b^2 + z^2)^{3/2}(b^2 + z'^2)^{3/2}} \times \langle 0 | \mathfrak{z}^2 | 0 \rangle , \qquad (2.16)$$

where $\mathfrak{z}$ denotes the sum of all the z coordinates of the bound electrons. Putting this expression into Eq. (2.15), we find

$$\chi_{\rm pol}(\vec{b}) = \frac{\langle 0 | \mathfrak{z}^2 | 0 \rangle}{kk' b^2} \int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy \times \frac{xy + 1}{(1 + x^2)^{3/2}(1 + y^2)^{3/2}} \sin\eta(x - y) , \qquad (2.17)$$

where $\eta = \xi b$. If we now insert this into expression (2.12) it will give a contribution to $f_{\rm OB}$, which we may denote by $f_{\rm OB}^{\rm pol}$. It is given by

$$f_{\rm OB}^{\rm pol} = \frac{k}{2\pi} \int d^2\vec{b}\, e^{i\vec{K}\cdot\vec{b}} \chi_{\rm pol}(\vec{b})$$

$$= \frac{\langle 0 | \mathfrak{z}^2 | 0 \rangle}{k'} \int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy \frac{xy + 1}{(1 + x^2)^{3/2}(1 + y^2)^{3/2}} \times \int_0^{\infty} J_0\left(\frac{K}{\xi}\eta\right) \frac{\sin\eta(x - y)}{\eta}\, d\eta . \qquad (2.18)$$

It is clear that for values of K such that $K \lesssim (\Delta/k)$, $f_{\rm OB}^{\rm pol}$ is of order k^{-1}. In fact, the integral involving the Bessel function can be evaluated analytically[23] to give

$$\Phi(t) \equiv \int_0^\infty J_0\left(\frac{K}{\xi}\eta\right) \frac{\sin\eta t}{\eta}\, d\eta = \begin{cases} \dfrac{\pi}{2}, & \dfrac{K}{\xi} \leq t \\ \sin^{-1}\dfrac{\xi}{K}t, & \dfrac{K}{\xi} \geq t, \end{cases} \tag{2.19}$$

so we may write

$$f_{\mathrm{OB}}^{\mathrm{pol}}(K) = \frac{\langle 0|\, \mathfrak{z}^2 |0\rangle}{k'} \int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy \times \frac{xy+1}{(1+x^2)^{3/2}(1+y^2)^{3/2}} \Phi(x-y)\ . \tag{2.20}$$

Integrating by parts and making a change of variables, we find

$$f_{\mathrm{OB}}^{\mathrm{pol}}(K) = \frac{\langle 0|\, \mathfrak{z}^2 |0\rangle}{k'} \left(\pi - \frac{K}{\xi} \int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^{3/2}} \int_0^{\pi/2} \frac{\sin\theta}{\{1+[x-(K/\xi)\sin\theta]^2\}^{1/2}}\, d\theta\right)\ .$$

This last integral can be done analytically with some difficulty to yield

$$f_{\mathrm{OB}}^{\mathrm{pol}} = \frac{\pi \langle 0|\, \mathfrak{z}^2 |0\rangle}{k} \left(1 - \frac{Ka}{[(Ka)^2+1]^{1/2}}\right), \tag{2.21}$$

where

$$a = k/2\Delta\ . \tag{2.22}$$

When K becomes larger than $a^{-1} = 2\Delta/k$, i.e., when $\theta > 2\,\Delta/k^2$, this term is of order $k^{-3}K^{-2}$ and is small compared to second-order static corrections to the real part of the amplitude, which are of order $k^{-2}K^{-2}$. However, for angles less than $2\,\Delta/k^2$ the contribution of Eq. (2.21) will provide the leading correction to the first Born approximation. It is interesting to note that in II we have evaluated the second Born scattering amplitude for atomic hydrogen and found [see Eq. (2.40a) of II]

$$\mathrm{Re}\bar{f}_{B2} = 2\pi \frac{K^2+8}{(K^2+4)^2} \left(\frac{1}{k} - \frac{K}{(k^2K^2+4\Delta^2)^{1/2}}\right) + O(k^{-2})\ . \tag{2.23}$$

For large k and small angles this expression reduces to

$$\mathrm{Re}\bar{f}_{B2} = \frac{\pi}{k}\left(1 - \frac{Ka}{[(Ka)^2+1]^{1/2}}\right),$$

which is in exact agreement with Eq. (2.21), since for hydrogen $\langle 0|\, \mathfrak{z}^2 |0\rangle = 1$.

In order to gain some physical insight into Eq. (2.21), let us use that equation to provide us with an effective potential $V_{\mathrm{pol}}(r)$, whose first Born term is given by Eq. (2.21). We have

$$V_{\mathrm{pol}}(r) = \frac{\langle 0|\, \mathfrak{z}^2 |0\rangle}{4\pi k} \int e^{-i\vec{K}\cdot\vec{r}} \left(1 - \frac{Ka}{[(Ka)^2+1]^{1/2}}\right) d\vec{K}$$
$$= -\frac{1}{ka^3\rho} \langle 0|\, \mathfrak{z}^2 |0\rangle \int_0^\infty \sin\rho q \times \left(1 - \frac{q}{(q^2+1)^{1/2}}\right) q\, dq\ , \tag{2.24}$$

where a is given by Eq. (2.22) and $\rho = r/a$. Integrating by parts twice, we have

$$V_{\mathrm{pol}}(r) = -\frac{1}{ka^3\rho^3} \langle 0|\, \mathfrak{z}^2 |0\rangle \times \left(3\int_0^\infty \frac{\sin\rho q}{(q^2+1)^{5/2}}\, dq - \int_0^\infty \frac{\sin\rho q}{(q^2+1)^{3/2}}\, dq\right)\ .$$

Integrals of this type can be evaluated analytically.[23] One finds

$$V_{\mathrm{pol}}(r) = -\frac{\pi}{2ka^3\rho} \langle 0|\, \mathfrak{z}^2 |0\rangle \times \left([I_0(\rho) - L_0(\rho)] - \frac{1}{\rho}[I_1(\rho) - L_1(\rho)]\right)\ , \tag{2.25}$$

where I_n is a modified Bessel function and L_n is a modified Struve function. Tables of $I_0 - L_0$ and $I_1 - L_1$ are available in the literature.[24] From $V_{\mathrm{pol}}(r)$, $\chi_{\mathrm{pol}}(b)$ can be obtained by numerical integration. Using the asymptotic expansions[24] of $I_0 - L_0$ and $I_1 - L_1$ the large-r behavior of $V_{\mathrm{pol}}(r)$ is readily obtained:

$$V_{\mathrm{pol}}(r) = -\frac{\bar{\alpha}}{2r^4}\left(1 + \frac{6a^2}{r^2} + \frac{135a^4}{r^4} + \cdots\right), \tag{2.26}$$

where

$$\bar{\alpha} = \frac{2\langle 0|\, \mathfrak{z}^2 |0\rangle}{\Delta} \tag{2.27}$$

is precisely the polarizability which would be obtained in the closure approximation.

The function $V_{\mathrm{pol}}(r)$ clearly has the polarization form, which we anticipated in our choice of notation. However, we note that at large r $V_{\mathrm{pol}}(r)$ lies below the asymptotic form $-\bar{\alpha}/2r^4$. This is just the opposite of what would be obtained from a Buckingham polarization potential of the form $-\bar{\alpha}/2(r^2+a^2)^2$. We may also remark that since a is proportional to k the correction term of relative order r^{-2} can be quite important, even for rather large values of r. Thus, for the case of helium at 500 eV, where $a \simeq 2.4$, the correction is more than 30% at $r = 10$.

The quantity of direct interest to us is $\chi_{\mathrm{pol}}(b)$, which can be determined from $V_{\mathrm{pol}}(r)$ by

$$\chi_{pol}(b) = -\frac{1}{k}\int_{-\infty}^{\infty} V_{pol}(b,z)\,dz\ . \qquad (2.28)$$

This is readily obtained by using either Eq. (2.24) or (2.25) for $V_{pol}(r)$. In either case, a simple numerical integration yields χ_{pol}.

Finally, with the phases χ_{st}, χ_{abs}, and χ_{pol} determined according to the above discussion, we use Eq. (2.11) to write

$$\chi_{opt} = \chi_{st} + \chi_{abs} + \chi_{pol}\ . \qquad (2.29)$$

This enables us to evaluate the optical eikonal and optical Born amplitudes given by Eqs. (2.10) and (2.12), respectively. The phases χ_{abs} and χ_{pol} are dominant in correcting the first Born approximation at small angles where virtual excitation channels have very large amplitudes. The static phase χ_{st} plays the dominant role at larger angles as the inelastic channels become unimportant compared to the elastic channel.

As we have already indicated in Eq. (2.23), the quantity $\mathrm{Re}\bar{f}_{B2}$ contains terms of order k^{-2} which a full wave treatment of the optical potential would give by the iteration of the static potential $V^{(1)}$ to second order. However, as we have pointed out elsewhere,[12,13] this contribution is not present in an eikonal treatment. Fortunately, at least for ground-state wave functions $|0\rangle$ of the Hartree-Fock type, it is a simple matter to obtain the second Born term $\mathrm{Re}\bar{f}^{\,st}_{B2}$ corresponding to the static potential $V^{(1)}$. Therefore we may add this term to the real part of our optical eikonal scattering amplitude (2.10). This gives us the *direct* amplitude for elastic scattering

$$f_d = f_{OE} + \mathrm{Re}\bar{f}^{\,st}_{B2}\ . \qquad (2.30)$$

With f_d determined in this way, and keeping in mind that k is large, it is clear that an expansion of f_d in powers of V will duplicate the Born series through second order. It will also give approximations to higher terms of the Born series ($\bar{f}_{B3}$, $\bar{f}_{B4}, \ldots$). The third-order contribution will be discussed in detail below for the case of electron-helium scattering.

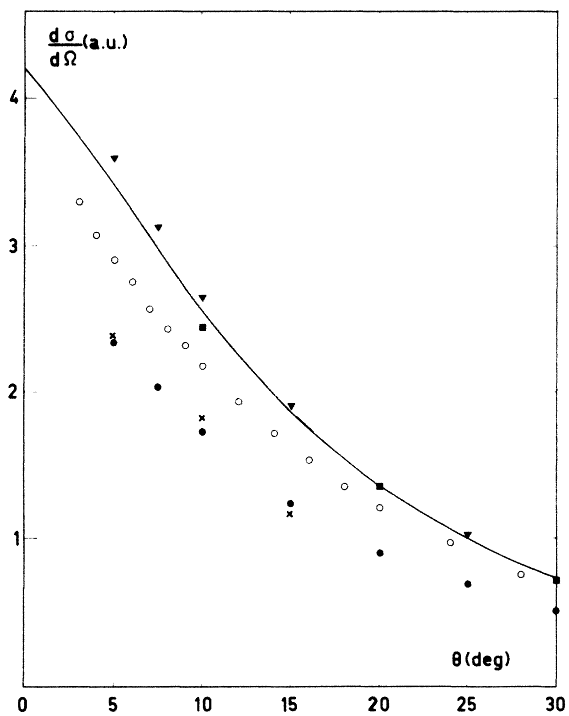

FIG. 1. Differential cross section (in a.u.) for elastic electron scattering by helium at 100 eV. The curve represents the results of this paper, using the optical eikonal method. Triangles are the experimental results of Vriens *et al*. (Ref. 26); solid circles are the same results renormalized by Chamberlain *et al*. (Ref. 16); squares show the data of Crooks and Rudd (Ref. 17); crosses display the results of Vuskovic (Ref. 18); open circles are the data of Jost *et al*. (Ref. 27).

C. Exchange scattering

As in II, we will treat exchange corrections only through leading order in k^{-1}. Therefore, we shall approximate the exchange amplitude g by g_{Och}, the Ochkur[25] approximation to it. For example, in the case of electron-helium scattering discussed in Sec. III we write the full optical elastic scattering amplitude as

$$f_{opt} = f_d - g_{Och}\ , \qquad (2.31)$$

so that the differential cross section for elastic scattering is given by $d\sigma_{opt}/d\Omega = |f_{opt}|^2$.

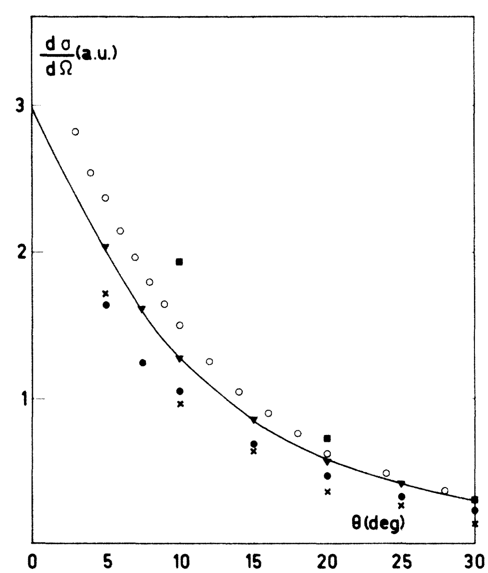

FIG. 2. Same as Fig. 1, but at an energy of 200 eV.

III. ELECTRON-HELIUM ELASTIC SCATTERING

A. Results and comparison with experiment

As an illustration of the theory presented in Sec. II, we now discuss in detail the case of electron-helium elastic scattering at incident energies between 100 and 500 eV, where recent absolute[15-18] and relative[26,27] experimental data are available. The ground-state wave function used in performing our calculations is the same as that used in II. With the quantity Δ determined (as in II) to be 1.3 a.u., we emphasize that this optical eikonal calculation contains *no* adjustable parameters. In a more complicated atom Δ should be regarded as a phenomenological parameter.

Our results are summarized in Figs. 1–4 and in Tables I and II. The former display small-angle results, while the tables give a picture of the scattering over the full angular range. These tables also contain a comparison with previous theoretical results of II and III. We note that the agreement between our results and the experimental data at angles such that $0° \leqslant \theta \leqslant 30°$ is excellent. The tables, however, reveal that at larger angles the optical-eikonal–model results are not so reliable. In particular, the static results of III, which are just a full wave treatment of the lowest-order (static) optical potential together with the leading (Ochkur) exchange correction, but with absorption and polarization terms omitted, agree much better with experiment than do the present optical eikonal results, which contain static, absorption, and polarization effects. The reason for this is twofold. First, one expects that at wide angles the effects of polarization and absorption will be small; second, as we noted in I–III the eikonal method is seriously deficient in dealing with higher-order terms in the Born series, which terms have their greatest importance precisely at large angles. In fact, the eikonal method omits at each order in k^{-1} a term of the same order in k^{-1} as the one which it includes. This omission is unimportant in strong-coupling cases, but in an intermediate-coupling regime such as that with which we are dealing here this omission can be serious. It is just this defect which made it necessary for us to add the term $\mathrm{Re}\bar{f}^{\,\mathrm{st}}_{B2}$ to the amplitude f_{OE} [see Eq. (2.30)]. Such an addition would not of course be necessary in a full wave treatment. We should remark here that Tables I and II suggest that in more complicated atoms a wave treatment of $V^{(1)}$ alone should give a good picture of elastic scattering outside the small-angle region.

In order to see when χ_{st}, χ_{abs}, and χ_{pol} play their important roles, let us consider in more detail

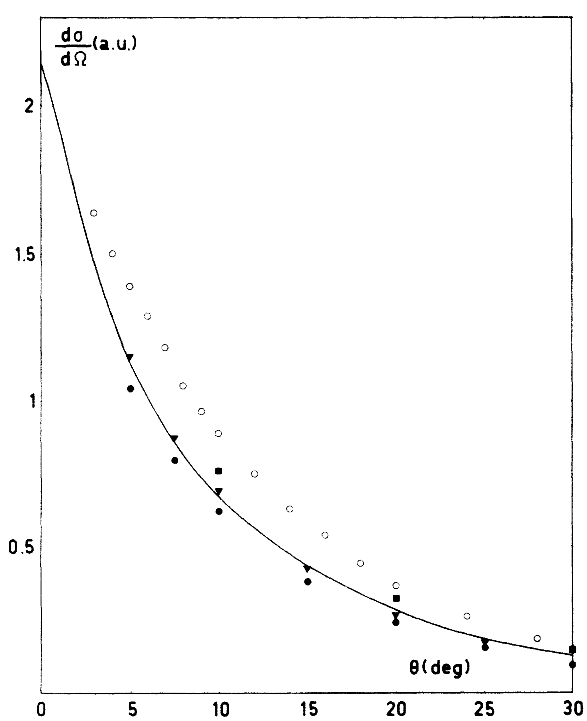

FIG. 3. Same as Fig. 1, but at an energy of 400 eV.

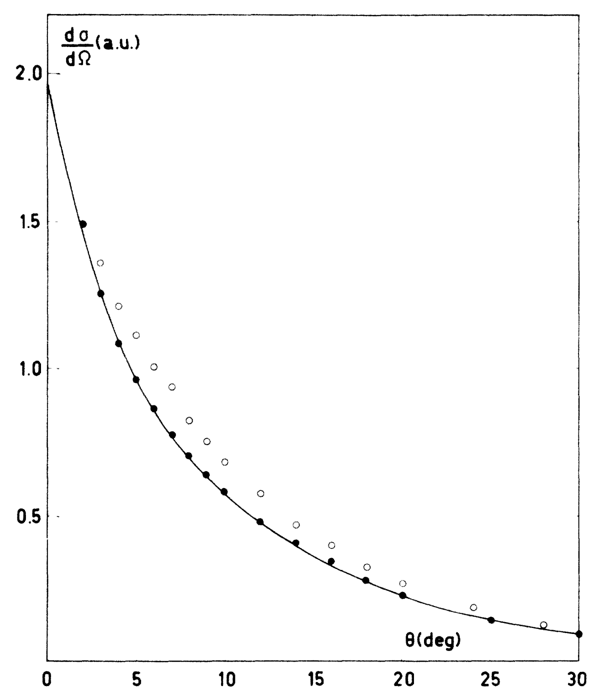

FIG. 4. Differential cross section (in a.u.) for elastic electron scattering by helium at 500 eV. The curve represents the result of this paper, using the optical eikonal method. Solid circles are the results of Bromberg (Ref. 15); open circles are the data of Jost *et al.* (Ref. 27).

TABLE I. Comparison of various theoretical and experimental differential cross sections for elastic electron-helium scattering at an incident-electron energy of 200 eV. All results are in units of a_0^2/ster.

	Theoretical Values			Experimental Values				
θ (deg)	Eikonal Born series (Ref. 14)	Static plus exchange (Ref. 20)	Optical eikonal	Vriens *et al.* (Ref. 26)	Chamberlain *et al.* (Ref. 16)	Crooks and Rudd (Ref. 17)	Vuskovic (Ref. 18)	Jost *et al.* (Ref. 27)
0	3.16	8.54 (−1)	2.97	···	···	···	···	···
5	2.12	8.22 (−1)	2.03	2.04	1.64	···	1.72	2.36
10	1.34	7.37 (−1)	1.28	1.28	1.04	1.93	9.63 (−1)	1.50
15	8.65 (−1)	6.21 (−1)	8.50 (−1)	8.36 (−1)	6.81 (−1)	···	6.38 (−1)	9.65 (−1)
20	5.83 (−1)	5.01 (−1)	5.81 (−1)	5.61 (−1)	4.58 (−1)	7.13 (−1)	3.63 (−1)	6.07 (−1)
25	4.06 (−1)	3.90 (−1)	4.08 (−1)	3.99 (−1)	3.25 (−1)	···	2.64 (−1)	4.45 (−1)
30	2.88 (−1)	2.99 (−1)	2.90 (−1)	2.75 (−1)	2.24 (−1)	3.25 (−1)	1.41 (−1)	3.20 (−1)
50	8.76 (−2)	1.03 (−1)	8.42 (−2)	···	···	1.03 (−1)	6.08 (−2)	1.00 (−1)
70	3.61 (−2)	4.23 (−2)	3.08 (−2)	···	···	4.23 (−2)	2.39 (−2)	4.11 (−2)
90	1.97 (−2)	2.17 (−2)	1.41 (−2)	···	···	2.33 (−2)	1.45 (−2)	2.00 (−2)
110	1.32 (−2)	1.34 (−2)	7.85 (−3)	···	···	1.41 (−2)	9.47 (−3)	1.21 (−2)
130	1.01 (−2)	9.64 (−3)	5.17 (−3)	···	···	1.05 (−2)	7.37 (−3)	8.57 (−3)
150	8.60 (−3)	7.81 (−3)	3.95 (−3)	···	···	8.43 (−3)	6.43 (−3)	···
180	7.88 (−3)	6.97 (−3)	3.41 (−3)	···	···	···	···	···

the importance of various contributions to that part of the optical eikonal amplitude which is quadratic in V[see Eq. (2.1)] and which we denote by $f_{\text{opt}}^{(2)}$. We remind the reader that $V^{(1)}$ is linear in V and $V^{(2)}$ is quadratic in V, so that $f_{\text{opt}}^{(2)}$ comes from χ_{st} acting in second-order perturbation theory (f_{opt}^{s2}), from χ_{abs} and χ_{pol} acting in first-order perturbation theory ($f_{\text{OB}}^{\text{abs}}$ and $f_{\text{OB}}^{\text{pol}}$, respectively) and from $\text{Re}\bar{f}_{B2}^{\text{st}}$, which we have added in Eq. (2.30). This amplitude should be nearly equal to the second Born amplitude $\bar{f}_{B2}$, which is just that part of the *exact* direct scattering amplitude which is quadratic in V; it is *not* the same as $\bar{f}_{\text{OE2}}$, which is the term in the optical eikonal amplitude quadratic in $\mathcal{V}_{\text{opt}}$.

Table III shows the real part of $f_{\text{opt}}^{(2)}$, along with the separate contributions of $f_{\text{OB}}^{\text{pol}}$ (which is purely real) and $\text{Re}\bar{f}_{B2}^{\text{st}}$ at an energy of 200 eV. Also included for comparison is $\text{Re}\bar{f}_{B2}$ as calculated in II. We see that for angles less than about 20° the part of $\text{Re}f_{\text{opt}}^{(2)}$ coming from $f_{\text{OB}}^{\text{pol}}$ dominates, but at larger angles $\text{Re}\bar{f}_{B2}^{\text{st}}$ controls the behavior of the second-order amplitude. Table IV illustrates a similar situation for $\text{Im}f_{\text{opt}}^{(2)}$. It shows the separate contributions of $\text{Im}f_{\text{OB}}^{\text{abs}}$ and $\text{Im}f_{\text{opt}}^{s2}$, and we see that the absorption part dominates at angles less than about 20°, whereas $\text{Im}f_{\text{opt}}^{s2}$ controls $\text{Im}f_{\text{opt}}^{(2)}$ at larger angles. We may remark that the angle at which $f_{\text{opt}}^{(2)}$ becomes dominated by $f_{\text{OB}}^{\text{abs}}$ and $f_{\text{OB}}^{\text{pol}}$ depends on energy and varies roughly as E^{-1}. We also note that for both $\text{Re}f_{\text{opt}}^{(2)}$ and $\text{Im}f_{\text{opt}}^{(2)}$ the agreement with $\text{Re}\bar{f}_{B2}$ and $\text{Im}\bar{f}_{B2}$ is quite good.

TABLE II. Same as Table I, but for an incident-electron energy of 400 eV.

	Theoretical Values			Experimental Values			
θ (deg)	Eikonal Born series (Ref. 14)	Static plus exchange (Ref. 20)	Optical eikonal	Vriens *et al.* (Ref. 26)	Chamberlain *et al.* (Ref. 16)	Crooks and Rudd (Ref. 17)	Jost *et al.* (Ref. 27)
0	2.24	7.39 (−1)	2.15	···	···	···	···
5	1.18	6.86 (−1)	1.14	1.15	1.04	···	1.39
10	6.89 (−1)	5.57 (−1)	6.75 (−1)	6.88 (−1)	6.22 (−1)	7.61 (−1)	8.93 (−1)
15	4.30 (−1)	4.11 (−1)	4.35 (−1)	4.20 (−1)	3.80 (−1)	···	5.82 (−1)
20	2.85 (−1)	2.85 (−1)	2.82 (−1)	2.62 (−1)	2.37 (−1)	3.17 (−1)	3.64 (−1)
25	1.84 (−1)	1.93 (−1)	1.83 (−1)	1.65 (−1)	1.49 (−1)	···	2.35 (−1)
30	1.23 (−1)	1.30 (−1)	1.20 (−1)	1.05 (−1)	9.48 (−2)	1.41 (−1)	1.55 (−1)
50	2.96 (−2)	3.22 (−2)	2.78 (−2)	···	···	3.34 (−2)	3.57 (−2)
70	1.09 (−2)	1.14 (−2)	9.29 (−3)	···	···	1.17 (−2)	1.21 (−2)
90	5.45 (−3)	5.34 (−3)	4.16 (−3)	···	···	6.60 (−3)	5.18 (−3)
110	3.37 (−3)	3.10 (−3)	2.33 (−3)	···	···	3.33 (−3)	3.00 (−3)
130	2.44 (−3)	2.12 (−3)	1.55 (−3)	···	···	2.32 (−3)	1.96 (−3)
150	2.00 (−3)	1.67 (−3)	1.20 (−3)	···	···	1.83 (−3)	···
180	1.80 (−3)	1.34 (−3)	1.04 (−3)	···	···	···	···

TABLE III. Contributions to the real part of the optical eikonal amplitude which are proportional to V^2. The real part of the second Born term is included for comparison. The incident-electron energy is 200 eV.

θ (deg)	f_{OB}^{pol}	$\mathrm{Re}\bar{f}_{B2}^{st}$	$\mathrm{Re}f_{OE}^{(2)} = f_{opt}^{pol} + \mathrm{Re}\bar{f}_{B2}^{st}$	$\mathrm{Re}\bar{f}_{B2}$
0	6.48 (−1)	6.31 (−2)	7.11 (−1)	7.31 (−1)
5	3.72 (−1)	6.27 (−2)	4.35 (−1)	4.34 (−1)
10	1.90 (−1)	6.19 (−2)	2.52 (−1)	2.47 (−1)
15	1.13 (−1)	6.03 (−2)	1.73 (−1)	1.55 (−1)
20	7.03 (−2)	5.84 (−2)	1.29 (−1)	1.11 (−1)
30	3.49 (−2)	5.34 (−2)	8.83 (−2)	7.79 (−2)
40	2.08 (−2)	4.78 (−2)	6.86 (−2)	6.42 (−2)
50	1.38 (−2)	4.22 (−2)	5.60 (−2)	5.43 (−2)
60	9.82 (−3)	3.70 (−2)	4.68 (−2)	4.62 (−2)
90	4.90 (−3)	2.55 (−2)	3.04 (−2)	2.95 (−2)
120	3.30 (−3)	1.92 (−2)	2.25 (−2)	2.13 (−2)
150	2.52 (−3)	1.62 (−2)	1.87 (−2)	1.75 (−2)
180	2.45 (−3)	1.53 (−2)	1.77 (−2)	1.65 (−2)

B. Discussion of higher-order terms

Let us now compare the term in our amplitude, f_{opt}, proportional to V^3 with the corresponding term in the Born series. By using an analysis similar to that of II it can be shown that for k large the dominant part of the V^3 contribution to that amplitude is the real part, namely,

$$\mathrm{Re}f_{opt}^{(3)} = \mathrm{Re}f_{opt}^{s3} + \mathrm{Re}f_{opt}^{sa}, \tag{3.1}$$

where we have set

$$\mathrm{Re}f_{opt}^{s3} = \frac{k}{2\pi i}\int d\vec{b}\, e^{i\vec{K}\cdot\vec{b}}\left(-\frac{i}{6}\chi_{st}^3\right) \tag{3.2}$$

and

$$\mathrm{Re}f_{opt}^{sa} = \frac{k}{2\pi i}\int d\vec{b}\, e^{i\vec{K}\cdot\vec{b}}\left(-\tfrac{1}{2}\chi_{st}\chi_{abs}\right). \tag{3.3}$$

We show in Table V the quantities $\mathrm{Re}f_{opt}^{s3}$, $\mathrm{Re}f_{opt}^{sa}$, and $\mathrm{Re}f_{opt}^{(3)}$ together with the real part of the third Born term $\mathrm{Re}\bar{f}_{B3}$ (as obtained[28] in II) for various scattering angles and an incident-electron energy of 200 eV. The agreement between $\mathrm{Re}f_{opt}^{(3)}$ and $\mathrm{Re}\bar{f}_{B3}$ is excellent for angles greater than about 30° and is seen to be poorest in the forward direction. It is worth noting that at all angles the term $\mathrm{Re}f_{opt}^{sa}$ makes a significant contribution to $\mathrm{Re}f_{opt}^{(3)}$. This contribution brings $\mathrm{Re}f_{opt}^{(3)}$ into good agreement with $\mathrm{Re}\bar{f}_{B3}$ outside the small-angle region. Thus the iteration of the second-order optical potential produces an important part of the third-order contribution to the scattering amplitude, with both static and absorption parts playing a significant role. The difficulties at small angles

TABLE IV. Contributions to the imaginary part of the optical eikonal amplitude which are proportional to V^2. The imaginary part of the second Born term is included for comparison. The incident-electron energy is 200 eV.

θ (deg)	$\mathrm{Im}f_{OB}^{abs}$	$\mathrm{Im}f_{opt}^{s2}$	$\mathrm{Im}f_{opt}^{(2)} = \mathrm{Im}f_{OB}^{abs} + \mathrm{Im}f_{opt}^{s2}$	$\mathrm{Im}\bar{f}_{B2}$
0	7.70 (−1)	2.29 (−1)	9.99 (−1)	8.84 (−1)
5	6.69 (−1)	2.28 (−1)	8.97 (−1)	7.97 (−1)
10	4.78 (−1)	2.26 (−1)	7.04 (−1)	6.28 (−1)
15	3.19 (−1)	2.22 (−1)	5.41 (−1)	4.79 (−1)
20	2.08 (−1)	2.17 (−1)	4.25 (−1)	3.73 (−1)
30	9.00 (−2)	2.05 (−1)	2.95 (−1)	2.57 (−1)
40	4.21 (−2)	1.90 (−1)	2.32 (−1)	2.05 (−1)
50	2.20 (−2)	1.75 (−1)	1.95 (−1)	1.78 (−1)
60	1.27 (−2)	1.60 (−1)	1.73 (−1)	1.60 (−1)
90	3.92 (−3)	1.25 (−1)	1.29 (−1)	1.24 (−1)
120	1.89 (−3)	1.03 (−1)	1.05 (−1)	1.03 (−1)
150	1.23 (−3)	9.16 (−2)	9.28 (−2)	9.15 (−2)
180	1.08 (−3)	8.81 (−2)	8.92 (−2)	8.81 (−2)

TABLE V. Comparison of the quantities $\mathrm{Re}f_{opt}^{s3}$, $\mathrm{Re}f_{opt}^{sa}$, $\mathrm{Re}f_{opt}^{(3)}$, and $\bar{f}_{B3}$ for electron-helium scattering at an incident energy of 200 eV.

θ (deg)	$\mathrm{Re}f_{opt}^{s3}$	$\mathrm{Re}f_{opt}^{sa}$	$\mathrm{Re}f_{opt}^{(3)}$	$\mathrm{Re}\bar{f}_{B3}$
0	−9.68 (−2)	−1.05 (−1)	−2.02 (−1)	−1.17 (−1)
10	−9.64 (−2)	−1.01 (−1)	−1.97 (−1)	−1.39 (−1)
20	−9.52 (−2)	−9.09 (−2)	−1.86 (−1)	−1.54 (−1)
30	−9.33 (−2)	−7.79 (−2)	−1.71 (−1)	−1.53 (−1)
60	−8.50 (−2)	−4.43 (−2)	−1.29 (−1)	−1.23 (−1)
90	−7.63 (−2)	−2.70 (−2)	−1.03 (−1)	−9.92 (−2)
120	−6.95 (−2)	−1.90 (−2)	−8.86 (−2)	−8.48 (−2)
150	−6.54 (−2)	−1.56 (−2)	−8.10 (−2)	−7.77 (−2)
180	−6.41 (−2)	−1.46 (−2)	−7.87 (−2)	−7.56 (−2)

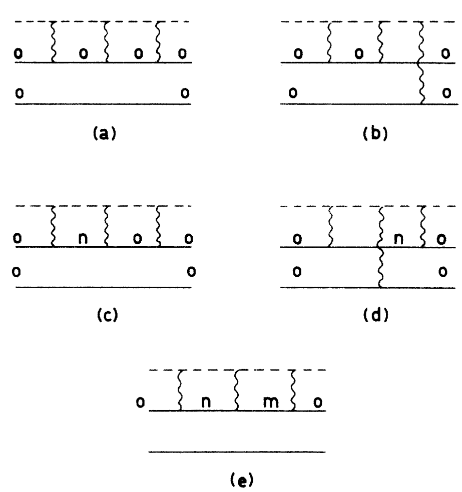

FIG. 5. Typical third-order diagrams contributing to the scattering amplitude. Figures 5(a) and 5(b) show, respectively, a connected and a disconnected part which contribute to $\mathrm{Re}f_{opt}^{s3}$. Figures 5(c) and 5(d) display, respectively, a connected and a disconnected term contributing to $\mathrm{Re}\,f_{opt}^{sa}$. Figure 5(e) is a disconnected diagram in which the target experiences two virtual excitations. Diagrams of the type (e) are not included in a second-order optical model. The indices o, n, and m refer to single-particle orbitals.

TABLE VI. Comparison of the real part of the scattering amplitude as calculated by three different approaches: the optical eikonal method, the eikonal Born series and dispersion relations.

E (eV)	Re $f_{\rm opt}(0)$	Re $f_{\rm EBS}(0)$ (Ref. 14)	Re $f_{\rm DR}(0)$ (Ref. 21)
100	1.68	1.91	1.91
150	1.54	1.67	1.81
200	1.44	1.54	1.71
300	1.32	1.39	1.48
400	1.25	1.30	1.36
500	1.21	1.24	1.29

with the third-order term are not surprising, in view of the fact that no second-order optical model can produce long-range forces in third order. Such effects can only arise by including a third-order contribution to the optical potential, i.e., by writing

$$\mathcal{V}_{\rm opt} = V^{(1)} + V^{(2)} + V^{(3)} . \qquad (3.4)$$

In order to analyze in more detail the structure of the optical eikonal third-order term $\mathrm{Re}f^{(3)}_{\rm opt}$, let us consider separately its components $\mathrm{Re}f^{s3}_{\rm opt}$ and $\mathrm{Re}f^{sa}_{\rm opt}$, given, respectively, by Eqs. (3.2) and (3.3). The term $\mathrm{Re}f^{s3}_{\rm opt}$ accounts for contributions in which the target remains in its ground state during all interactions. In fact, using a single-particle picture to describe the target, this term may be considered as a sum of connected and disconnected parts of the type shown in Figs. 5(a) and (b). On the other hand, the term $\mathrm{Re}f^{sa}_{\rm opt}$ takes into account the contributions in which the target experiences a single virtual excitation during all interactions. This term also contains connected and disconnected parts, of the type shown in Figs. 5(c) and (d). We note that the contributions in which the target experiences two virtual excitations are not included in our model. These contributions come entirely from disconnected parts, typified by Fig. 5(c). In higher orders of perturbation theory it is clear from this analysis that the second-order optical model will miss all terms containing two virtual excitations. Among such missing contributions are those due to elastic scattering in virtual excited states, which are responsible for long-range forces in higher orders.

Finally, let us remark that the optical Born results, obtained by using the quantity $f_{\rm OB}$ [Eq. (2.12)] instead of $f_{\rm OE}$, do not contain terms of higher than second order (in the coupling constant) and are distinctly inferior to the values obtained from the optical eikonal theory.

C. Comparison with dispersion relations

As a final test of our optical eikonal calculations, let us compare the real part of our full amplitude $f_{\rm opt}$ [given by Eq. (2.31)] in the forward direction with the values obtained by Bransden and McDowell[21] using experimental data and dispersion relations. This comparison is made in Table VI, where we also display the results of our EBS calculations.[14] We note that our results agree well with the dispersion-relation calculations, the optical eikonal values being smaller than those of Bransden and McDowell by about 15% at the lowest energies and less than 7% at the higher energies. As we already pointed out in Sec. III B, the optical eikonal results for $\mathrm{Re}f_{\rm opt}$ $(\theta=0)$ lie consistently below the corresponding EBS values, but the disagreement in this case is smaller, being only of the order of 4% or less at energies above 300 eV.

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†Fulbright Research Scholar, on leave for the academic year 1973–74 at the Université Libre de Bruxelles.

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

[2]M. H. Mittleman, Ann. Phys. (N. Y.) 14, 94 (1961); in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic, New York, 1965), Vol. 1, p. 183.

[3]M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964), Chap. 11; A. L. Fetter and K. M. Watson, in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic, New York, 1965), Vol. 1, p. 115.

[4]R. T. Pu and E. Chang, Phys. Rev. 151, 31 (1966).

[5]H. P. Kelly, Phys. Rev. 160, 44 (1967); Phys. Rev. 166, 47 (1968); Phys. Rev. 171, 54 (1968).

[6]B. Schneider, H. S. Taylor, and R. Yaris, Phys. Rev. A 1, 855 (1970).

[7]J. E. Purcell, R. A. Berg, and A. E. S. Green, Phys. Rev. A 2, 107 (1970); P. S. Ganas, S. K. Dutta, and A. E. S. Green, Phys. Rev. A 2, 111 (1970).

[8]M. H. Mittleman, Phys. Rev. A 2, 1846 (1970).

[9]C. J. Joachain and M. H. Mittleman, Phys. Lett. 36A, 209 (1971).

[10]C. J. Joachain and M. H. Mittleman, Phys. Rev. A 4, 1492 (1971).

[11] R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin (Interscience, New York, 1959), Vol. 1, p. 315.

[12] F. W. Byron, Jr. and C. J. Joachain, Physica 66, 33 (1973).

[13] F. W. Byron, Jr., C. J. Joachain, and E. H. Mund, Bull. Am. Phys. Soc. 17, 542 (1972); Phys. Rev. D 8, 2622 (1973). This paper will be referred to as I.

[14] F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. A 8, 1267 (1973). This paper will be referred to as II.

[15] J. P. Bromberg, J. Chem. Phys. 50, 3906 (1969).

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

[17] G. B. Crooks and M. E. Rudd, Bull. Am. Phys. Soc. 17, 131 (1972); G. B. Crooks, thesis (University of Nebraska, 1972) (unpublished).

[18] L. D. Vuskovic, thesis (Institute for Physics, Beograd, 1972) (unpublished).

[19] Y. K. Kim and M. Inokuti, Phys. Rev. 165, 39 (1968).

[20] F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. A 8, 3266 (1973). This paper will be referred to as III.

[21] B. H. Bransden and M. R. C. McDowell, J. Phys. B 3, 29 (1970).

[22] Because of our choice of atomic units to express all quantitites (including energies), some of our formulas differ slightly from the corresponding ones in Ref. 10.

[23] See, for example, I. S. Gradshteyn and I. W. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965).

[24] See, for example, *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun, Natl. Bur. Std. Applied Mathematic Series No. 55 (U. S. GPO, Washington, D. C., 1964).

[25] V. I. Ochkur and V. F. Brattsev, Opt. Spectr. 19, 274 (1965).

[26] L. Vriens, C. E. Kuyatt, and S. R. Mielczarek, Phys. Rev. 170, 163 (1968).

[27] K. Jost, M. Fink, and P. Herrmann, in *Abstracts of Papers of the Eighth International Conference on the Physics of Electron-Atom Collisions*, edited by B. C. Cobic and M. V. Kurepa (Institute of Physics, Beograd, 1973), Vol. 1, p. 277; Phys. Rev. A (to be published).

[28] As shown in II, Re $\bar{f}_{B3}$ may be approximated by its Glauber value, $\bar{f}_{G3}$ at least for processes in which there is no change in the internal angular momentum of the target.