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Excitation of Atomic Hydrogen and Helium in the Eikonal Approximation

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Some of the key approximations involved in the application of the eikonal method to atomic physics are analyzed, and the method is related to the close-coupling approach. The importance of an accurate treatment of kinematics is stressed, and a Monte Carlo integration technique is used to facilitate the application of eikonal equations without simplifying kinematical assumptions. Results are presented on the excitation of the $2\,^1P$ state of helium by electron impact, on the excitation of the $2p$ state of atomic hydrogen by electron impact, and on the excitation of the $2s$ state of hydrogen by electron and positron (or proton) impact. Detailed comparison with experiment is made wherever possible.

I. INTRODUCTION

The purpose of this paper is to comment on an approximation, usually referred to as the Glauber approximation,[1] which has been in the past few years used to study electron-atom scattering.[2–5] In order to make connection with a more familiar approach, we may characterize this as a close-coupling method in which all channels are included at the expense of making certain approximations in each channel. This is to be contrasted with the approach of Burke, Schey, and Smith,[6] in which only a small number of channels are included but they are treated exactly. In systems such as $e+\mathrm{H}$ or $e+\mathrm{He}$, where the polarizability sum rule is known to saturate very slowly, this is a questionable approximation, and one might well hope that a technique which includes an infinite number of channels, even in an approximate way, could present a significant improvement.

The key approximations which go into the Glauber approach are

$$k_i a_i \gg 1 , \tag{1a}$$

$$E_i \gg \overline{V} , \tag{1b}$$

and

$$a_0 \Delta/\hbar v_1 \ll 1 , \tag{2}$$

where k_i is the incident projectile's momentum, E_i is its energy, $\overline{V}$ is a typical potential strength which occurs in the problem, Δ is a typical energy difference occurring in the spectrum of the target, and v_i. is the incident velocity of the projectile. If all quantities are expressed in atomic units, one sees that these three requirements are roughly equivalent. However, as one gets to the borderline of validity of the approximation, it may be useful to distinguish between them. We have separated Eq. (2) from Eqs. (1) because the role of energy differences between states is particularly important in electron-atom scattering, since the long range of the Coulomb potential means that these energy differences are crucial in guaranteeing that "optically-allowed" transitions have finite cross sections in electron-atom collisions. We shall look at this point in particular detail in what follows.

We shall begin in Sec. II by deriving some results in the close-coupling spirit utilizing only Eqs. (1a) and (1b), which we will refer to as the "eikonal approximation." Then we shall attempt to check the validity of this approximation in e-H scattering by comparison with exact results obtained by Burke *et al.*[6] Next, the assumption of Eq. (2)—the Glauber approximation—will be introduced and, after commenting further on the nature of the momentum transfer problem, we will use the Glauber approximation, without any of the usual auxiliary assumptions about the momentum transfer, to analyze certain key problems in e-H and e-He inelastic scattering.

II. EIKONAL-CLOSE-COUPLING APPROXIMATION

We will keep the discussion in this section as general as possible, rather than specialize to electron-atom collisions. Let us consider the collision of two composite systems whose internal coordinates will be denoted collectively by $\vec{r}$. The vector joining their centers of mass will be denoted by $\vec{R}$. We will write the interaction between the two systems as $(e^2/a_0)\,V(\vec{R},\vec{r})$, recognizing that we will be dealing exclusively with Coulomb interactions. Exchange effects will be neglected.

The Green's function for the "unperturbed" problem will have the form

$$G_0(\vec{R},\vec{R}',\vec{r},\vec{r}',E)=\sum_{\vec{k},m}\frac{e^{i\vec{k}\cdot(\vec{R}-\vec{R}')}\phi_m(\vec{r})\phi_m^*(\vec{r}')}{(2\pi)^3(\hbar^2k^2/2M+\epsilon_m-E-i\delta)} ,$$

where M is the reduced mass of the projectile and the integral sum represents an integral over $\vec{k}$ and also, in principle, over the continuous part of the spectrum of the internal degrees of freedom of the composite particles, as well as a sum over their discrete spectrum. $\phi_m(\vec{r})$ is the internal wave

function of the composite system, m denoting, in general, a collection of quantum numbers.

We may write for the total scattering wave function which corresponds to center-of-mass incident momentum $\vec{k}_i$ and initial internal state n

$$\Psi_{E_n}(\vec{R},\vec{r}) = e^{i\vec{k}_i\cdot\vec{R}}\phi_n(\vec{r}) - \frac{e^2}{a_0}\int G_0(\vec{R},\vec{R}',\vec{r},\vec{r}',E_n) \times V(\vec{R}',\vec{r}')\,\Psi_{E_n}(\vec{R}',\vec{r}')\,d\vec{R}'\,d\vec{r}' \ , \quad (3)$$

where $E_n = \hbar^2 k_i^2/2M + \epsilon_n$. In the close-coupling spirit, let us now replace the sum integral over the internal degrees of freedom by summing only on an index set I. Of course, in principle, I should contain all states, but this will not, in general, be practical, as we shall see later. Thus $\Psi_{E_n}(\vec{R},\vec{r})$ can be written in the form

$$\Psi_{E_n}(\vec{R},\vec{r}) = \sum_{m\in I} f_m^{(n)}(\vec{R})\phi_m(\vec{r}) \ . \quad (4)$$

Inserting this expression for the total wave function into Eq. (3), we obtain the following equation for $f_m^{(n)}(\vec{R})$:

$$f_m^{(n)}(\vec{R}) = \delta_{nm}e^{i\vec{k}_i\cdot\vec{R}} - \frac{e^2}{8\pi^3 a_0}\sum_{m'\in I}\int \frac{e^{i\vec{k}\cdot(\vec{R}-\vec{R}')}\,d\vec{k}}{\hbar^2k^2/2M + \epsilon_m - \hbar^2k_i^2/2M - \epsilon_n - i\delta}\,\mathcal{V}_{mm'}(\vec{R}')f_{m'}^{(n)}(\vec{R}')\,d\vec{R}'$$

for all $m\in I$. Here we have defined the dimensionless quantity

$$\mathcal{V}_{mm'}(\vec{R}) = \int \phi_m^*(\vec{r})\,V(\vec{R},\vec{r})\phi_{m'}(\vec{r})\,d\vec{r} \ . \quad (5)$$

If we define further

$$\Delta_{mn} = (2M/\hbar^2)(\epsilon_m - \epsilon_n) \ , \quad (6)$$

and make the eikonal ansatz

$$f_m^{(n)}(\vec{R}) = e^{i\vec{k}_i\cdot\vec{R}}\chi_m^{(n)}(\vec{R}) \ , \quad (7)$$

then we obtain the following equation for $\chi_m^{(n)}(\vec{R})$:

$$\chi_m^{(n)}(\vec{R}) = \delta_{mn} - \frac{\mathfrak{M}}{4\pi^3 a_0^2}\sum_{m'\in I}\int \frac{e^{i\vec{q}\cdot(\vec{R}-\vec{R}')}\,d\vec{q}}{q^2 + 2\vec{k}_i\cdot\vec{q} + \Delta_{mn} + i\delta}\,\mathcal{V}_{mm'}(\vec{R}')\chi_{m'}^{(n)}(\vec{R}')\,d\vec{R}', \quad (8)$$

where we have made the change of variable $\vec{q} = \vec{k} - \vec{k}_i$. $\mathfrak{M}$ is the reduced mass in units of the electron mass. Since we expect values of q of the order of magnitude of $1/a_0$ to be important in Eq. (8), and since $k_i \gg 1/a_0$, we rewrite Eq. (8) as

$$\chi_m^{(n)}(R) = \delta_{mn} - \frac{\mathfrak{M}}{8\pi^3 a_0^2 k_i}\sum_{m'\in I}\int e^{iq_x(X-X')}\frac{e^{iq_y(Y-Y')}e^{iq_z(Z-Z')}}{q_z + \Delta_{mn}/2k_i - i\delta} \times \left(1 + \frac{q^2}{2k_i q_z + \Delta_{mn} - i\delta}\right)^{-1} \mathcal{V}_{mm'}(\vec{R}')\chi_{m'}(\vec{R}')\,dX'\,dY'\,dZ'\,dq_x\,dq_y\,dq_z \ .$$

We now utilize Eq. (1a) to expand the term in large parenthesis. Because of Eq. (1a) it is clear that the second term in the expansion will be small compared to the first term, in fact, of order $1/k_i a_0$. However, it is easy to see that the second term is of absolute order $\mathcal{V}_{mm'}/E_i$. Since we expect on physical grounds that all the quantities we will be dealing with (the $\chi_m^{(n)}$) will be oscillatory in nature with absolute magnitude unity, it is important that terms neglected should be negligible compared to 1. Thus, if we assume Eq. (1b) to hold, we can neglect the second term in the expansion, but only if Eq. (1b) holds—Eq. (1a) is not sufficient.

Throwing away all but the leading term, we now can perform the q_x and q_y integrations (obtaining δ functions) and also the q_z integration, making use of the relation

$$\int_{-\infty}^{\infty}\frac{e^{iq\rho}}{q - i\delta}\,dq = \begin{cases} 2\pi i & \text{if } \rho > 0 \\ 0 & \text{if } \rho < 0 \end{cases} \ .$$

Integrating the two resultant δ-function integrals, we obtain

$$\chi_m^{(n)}(\vec{R}) = \delta_{mn} - \frac{\mathfrak{M}i}{k_i a_0^2}\sum_{m'\in I}\int_{-\infty}^{Z} e^{iq_{mn}(Z-Z')} \times \mathcal{V}_{mm'}(X,Y,Z')\chi_{m'}^{(n)}(X,Y,Z')\,dZ' \ , \quad (9)$$

where

$$q_{mn} \equiv \Delta_{mn}/2k_i = M(\epsilon_m - \epsilon_n)/\hbar^2 k_i \ . \quad (10)$$

In order to simplify Eq. (9), we define $\alpha_m^{(n)}(X,Y,Z)$ by

$$\chi_m^{(n)}(X,Y,Z) = e^{-iq_{mn}Z}\,\alpha_m^{(n)}(X,Y,Z) \quad (11)$$

and obtain for $\alpha_m^{(n)}$ the following expression:

$$\alpha_m^{(n)}(X,Y,Z) = \delta_{mn} - \frac{\mathfrak{M}i}{k_i a_0^2}\sum_{m'\in I}\int_{-\infty}^{Z} \mathfrak{U}_{mm'}(X,Y,Z')$$

$$\times \alpha_{m'}^{(n)}(X, Y, Z')\, dZ' , \qquad (12)$$

where

$$\mathfrak{U}_{mm'} = e^{iq_{mm'}Z} v_{mm'} . \qquad (13)$$

Note that the Volterra integral equation of Eq. (12) is equivalent to the differential equation

$$\frac{d\alpha_m^{(n)}(X, Y, Z)}{dZ} = -\frac{\mathfrak{M}i}{k_i a_0^2} \sum_{m' \in I} \mathfrak{U}_{mm'}(X, Y, Z)\alpha_{m'}^{(n)}(X, Y, Z), \qquad (14)$$

subject to the boundary condition

$$\alpha_m^{(n)}(X, Y, Z = -\infty) = \delta_{mn} . \qquad (15)$$

For most practical work, Eq. (14) is very useful since it lends itself readily to standard numerical techniques. Of course, if we truncate the sum in Eq. (14) so that only the single index n is contained in I, then the equation can be solved exactly. However, in general, a useful exact solution is not possible.

Now, in terms of $\alpha_m^{(n)}(\vec{R})$, the total wave function has the form [according to Eqs. (4), (7), and (11)]

$$\Psi_{E_n}(\vec{R}, \vec{r}) = e^{ik_i Z} \sum_{m \in I} e^{-iq_{mn}Z} \alpha_m^{(n)}(\vec{R})\phi_m(\vec{r}) . \qquad (16)$$

Using this expression, let us now look at the equation for the scattering amplitude:

$$T_{if} = -\frac{Me^2}{2\pi\hbar^2 a_0} \langle \phi_f | V | \Psi_i \rangle ,$$

where

$$\phi_f = e^{i\vec{k}_f \cdot \vec{R}} \phi_{n'}(\vec{r})$$

and Ψ_i is given by Eq. (16). Thus we have

$$T_{if} = -\frac{\mathfrak{M}}{2\pi a_0^2} \int e^{i(\vec{k}_i - \vec{k}_f)\cdot\vec{R}} \times \sum_{m \in I} e^{-iq_{mn}Z} v_{n'm}(\vec{R})\alpha_m^{(n)}(\vec{R})\, d\vec{R} . \qquad (17a)$$

But

$$e^{-iq_{mn}Z} = e^{iq_{nm}Z} = e^{iq_{nn'}Z} e^{iq_{n'm}Z} ,$$

so we have

$$T_{if} = -\frac{\mathfrak{M}}{2\pi a_0^2} \int e^{i(\vec{k}_i - \vec{k}_f)\cdot\vec{R}} e^{iq_{nn'}Z} \times \sum_{m \in I} \mathfrak{U}_{n'm}(\vec{R})\, \alpha_m^{(n)}(\vec{R})\, d\vec{R} . \qquad (17b)$$

But $\vec{k}_i \cdot \vec{R} + q_{nn'}Z = (k_i + q_{nn'})Z$. Now by conservation of energy

$$\hbar^2 k_i^2/2M + \epsilon_n = \hbar^2 k_f^2/2M + \epsilon_{n'} ,$$

from which we conclude that

$$k_f = k_i \left[1 + 2M(\epsilon_n - \epsilon_{n'})/\hbar^2 k_i^2\right]^{1/2}$$

$$\cong k_i + M(\epsilon_n - \epsilon_{n'})/\hbar^2 k_i = k_i + q_{nn'} ,$$

if we assume that typical bombarding energies are large compared with atomic excitation energies [this is equivalent to Eq. (1b) in atomic physics]. Thus we have

$$\vec{k}_i \cdot \vec{R} + q_{nn'}Z = (k_i + q_{nn'})Z = k_f Z = \vec{k}_i' \cdot \vec{R} ,$$

where $\vec{k}_i'$ is a vector in the Z direction whose magnitude is k_f. Hence, Eq. (17b) becomes

$$T_{if} = -\frac{\mathfrak{M}}{2\pi a_0^2} \int e^{i(\vec{k}_i' - \vec{k}_f)\cdot\vec{R}} \sum_{m \in I} \mathfrak{U}_{n'm}(\vec{R})\, \alpha_m^{(n)}(\vec{R})\, d\vec{R} . \qquad (18)$$

Since $|\vec{k}_i'| = |\vec{k}_f|$, Eq. (18) has the appearance of an *elastic* scattering amplitude, and we may use the familiar argument[7] which tells us that, for important scattering angles, $\vec{k}_i' - \vec{k}_f$ is nearly perpendicular to the Z axis [to be precise, for all scattering angles θ which satisfy $\theta \ll (2/k_f a_0)^{1/2}$]. Note that this result would not generally follow if we had $(\vec{k}_i - \vec{k}_f)$ instead of $(\vec{k}_i' - \vec{k}_f)$. Thus, we shall use cylindrical integration coordinates and write $\vec{R} = (\vec{b}, Z)$, where $\vec{b}$ is a two-dimensional vector in the XY plane. Let us write in Eq. (18)

$$e^{i(\vec{k}_i - \vec{k}_f)\cdot\vec{R}} \cong e^{i(\vec{k}_i - \vec{k}_f)\cdot\vec{b}} ,$$

so Eq. (18) becomes

$$T_{if} = \frac{\mathfrak{M}}{2\pi a_0^2} \int e^{i(\vec{k}_i' - \vec{k}_f)\cdot\vec{b}} \times \left(\sum_{m \in \alpha} \int_{-\infty}^{\infty} \mathfrak{U}_{n'm}(\vec{b}, Z)\alpha_m^{(n)}(\vec{b}, Z)\, dZ \right) d\vec{b} .$$

Looking back at our basic integral equation, Eq. (12), we see that the quantity in large parentheses has a very simple expression. Using Eq. (12), we obtain

$$T_{if} = \frac{k_i}{2\pi i} \int e^{i(\vec{k}_i' - \vec{k}_f)\cdot\vec{b}} [\alpha_{n'}^{(n)}(\vec{b}, Z = \infty) - \delta_{nn'}]\, d\vec{b} . \qquad (19)$$

The evaluation of the scattering amplitude now involves only the solution of the set of coupled differential equations given by Eq. (14). The n'th element of the column vector of solutions to Eq. (14) goes into Eq. (19), and a two-dimensional integration must be done to give the scattering amplitude. Note that $\alpha_{n'}^{(n)}(\vec{b}, Z)$ is needed only in the limit $Z \to \infty$, not for all Z. In most cases of interest, the dependence of $\alpha_{n'}^{(n)}(\vec{b}, Z = \infty)$ on the angle of orientation of $\vec{b}$ can be extracted explicitly from Eq. (14) in the form $e^{i\mu\phi}$. Then the ϕ integration in Eq. (19) can be done in closed form, yielding a Bessel function of the first kind.

If differential cross sections are not needed, then one can bypass Eq. (19) altogether and obtain a very simple expression for the cross section $\sigma_{nn'}$:

$$\sigma_{nn'} = (k_f/k_i)\int |T_{if}|^2 \, d\Omega \,,$$

where T_{if} is given by Eq. (19). Using Eq. (19) and calling $\vec{\Delta} = \vec{k}_i - \vec{k}_f$, we have

$$\sigma_{nn'} = \frac{k_i k_f}{(2\pi)^2} \int\int\int e^{i\vec{\Delta}\cdot(\vec{b}-\vec{b}')} \, [\alpha_{n'}^{(n)}(\vec{b}) - \delta_{nn'}] \times [\alpha_{n'}^{(n)*}(\vec{b}') - \delta_{nn'}] \, d\vec{b} \, d\vec{b}' \, d\Omega \,.$$

Here we have written $\alpha_{n'}^{(n)}(\vec{b}, Z=\infty)$ simply as $\alpha_{n'}^{(n)}(\vec{b})$. Now $d\Omega = \sin\theta \, d\theta \, d\phi$, where (θ, ϕ) defines the direction of the vector $\vec{k}_f$. But $\Delta^2 = k_i^2 + k_f^2 - 2k_i k_f \cos\theta$ and since $|\vec{k}_i| = k_f$, we have $\Delta^2 = 2k_f^2(1-\cos\theta)$, and therefore $\Delta d\Delta = k_f^2 \sin\theta \, d\theta$. Thus, we can write

$$\sigma_{nn'} = \frac{k_i}{(2\pi)^2 k_f} \int d\vec{b} \int d\vec{b}' \int_0^{2k_f}\int_0^{2\pi} e^{i\vec{\Delta}\cdot(\vec{b}-\vec{b}')} \times [\alpha_{n'}^{(n)}(\vec{b}) - \delta_{nn'}][\alpha_{n'}^{(n)*}(\vec{b}') - \delta_{nn'}] \, \Delta d\Delta d\phi \,.$$

Now $2k_f$ will, according to our assumptions, be a large number ($\gg 1/a_0$ in atomic units), so we can effectively consider the upper limit of the Δ integration to be infinity. Therefore, our expression for $\sigma_{nn'}$ becomes

$$\sigma_{nn'} = \frac{1}{(2\pi)^2}\left(\frac{k_i}{k_f}\right)\int d\vec{b} \int d\vec{b} \int d\vec{\Delta} e^{i\vec{\Delta}\cdot(\vec{b}-\vec{b}')} \times [\alpha_{n'}^{(n)}(\vec{b}) - \delta_{nn'}][\alpha_{n'}^{(n)*}(\vec{b}') - \delta_{nn'}] \,,$$

where the integral on $d\vec{\Delta}$ ranges over the entire two-dimensional plane. The integral yields $(2\pi)^2\delta(\vec{b}-\vec{b}')$ Finally, doing the integration on $\vec{b}'$, we have

$$\sigma_{nn'} = (k_i/k_f)\int |\alpha_{n'}^{(n)}(\vec{b}) - \delta_{nn'}|^2 d\vec{b} \,. \qquad (20)$$

Thus, in the eikonal approximation, the total cross sections, both elastic and inelastic, can be obtained directly, without looking at the differential cross sections. For inelastic processes, $\delta_{nn'} = 0$. Therefore we have

$$\sigma_{nn'}^{(\mathrm{inel})} = \frac{k_i}{k_f}\int |\alpha_{n'}^{(n)}(\vec{b})|^2 d\vec{b} \,. \qquad (21)$$

As remarked above, in most cases of interest the ϕ dependence of $\alpha_{n'}^{(n)}(\vec{b})$ has the form of a phase factor, so the ϕ integration in Eq. (21) is trivial, giving just a factor of 2π. Note that if we had calculated transition probabilities by working in a time-dependent straight-line-trajectory model, we would have obtained for $\sigma_{nn'}^{(\mathrm{inel})}$ Eq. (21) without the factor k_i/k_f. We will discuss this point further in Sec. III.

III. TEST OF EIKONAL HYPOTHESIS

The results which we have obtained for a coupled system described by the index set I are very easy to use if I contains only a few states. The most obvious domain of applicability of Eqs. (1a) and (1b), which have been basic to our work above, is certainly in heavy-particle–heavy-particle collisions. For example, consider the simple system $H^+ + H$ at energies greater than 1 kV. We clearly have $E_i \gg \overline{V}$, taking a typical potential strength conservatively to be about 1 a.u. (27.2 eV), and since $k_i a_0 = (2M_p a_0^2 E_i/\hbar^2)^{1/2}$, if E_i is greater than 1 kV $k_i a_0$ will always be greater than 100. In fact, even for energies significantly less than 1 kV, Eqs. (1a) and (1b) will be adequately satisfied.

The only difficulty which prevents the close-coupling eikonal approximation from being a panacea for heavy-particle–heavy-particle collisions (apart from purely technical matters concerning the use of complicated bound-state wave functions) is the tricky question of how many states should be included in I. It would not be useful to go into this question in detail here; suffice it to say that in many cases the number of states necessary to give useful results will be prohibitively large.

In this paper, we are concerned with electron-atom scattering, and it is this domain that we wish to test the assumptions of Eqs. (1a) and (1b). For electrons with energies from 50–100 eV, these assumptions are, at least formally, only marginally satisfied. When $E_i = 50$ eV, $k_i a_0 \simeq 2$ and $\overline{V}/E_i \simeq \frac{1}{2}$, again taking $\overline{V} \simeq 1$ a.u. When $E_i = 100$ eV, $k_i a_0 \simeq 3$ and $\overline{V}/E_i \simeq \frac{1}{4}$. Thus, Eqs. (1a) and (1b) are not impressively satisfied. However, a much more practical approach would be to test an exact solution of a finite close-coupled system against an eikonal–close-coupling solution. The two-collision configurations $e^- + H$ and $e^+ + H$ are ideal candidates, since Burke and his co-workers have expended considerable effort to obtain exact solutions for these problems in a finite-state close-coupling framework.

Since we merely wish to test hypotheses, let us look at the relatively simple five-state close-coupled system: $1s$-$2s$-$2pm$. The matrix elements which go into Eq. (14) are trivially evaluated in this case (because of symmetry considerations, there are only six matrix elements needed). Also, by symmetry, the ϕ dependence of the amplitudes can be displayed explicitly:

$$\alpha_{nlm}^{(1s)}(b, \phi, Z) = \beta_{nlm}^{(1s)}(b, Z) e^{-im\phi} \,,$$

so that Eq. (14) becomes

$$\frac{d\beta_{nlm}^{(1s)}(b, Z)}{dZ} = -\frac{\mathfrak{M}i}{k_i a_0^2} \times \sum_{n', l', m'} \mathfrak{W}_{nlm, n'l'm'}(b, Z) \beta_{n', l', m'}^{(1s)}(b, Z) \,, \qquad (22)$$

with $\beta_{100}^{(1s)}(b, Z=-\infty) = 1$ and $\beta_{nlm}^{(1s)}(b, Z=-\infty) = 0$ for $n \neq 1$. $\mathfrak{W}_{nlm, n'l'm'}$ is just equal to $\mathfrak{U}_{nlm, n'l'm'}$ with ϕ set equal to zero. Equation (22) must be solved for a range of values of b. This set of five coupled equa-

TABLE I. Comparison of eikonal- and exact-close-coupling results with kinematical simplifications.

Initial-final state	Born	Eikonal-Born	Exact close coupling (e^- + H)	Eikonal close coupling (e^- + H)	Exact close coupling (e^+ + H)	Eikonal close coupling (e^+ + H)
$1s2s$	$0.102\pi a_0^2$	$0.114\pi a_0^2$	$0.101\pi a_0^2$	$0.107\pi a_0^2$	$0.138\pi a_0^2$	$0.199\pi a_0^2$
$1s2p_+$	$0.283\pi a_0^2$	$0.378\pi a_0^2$	$0.239\pi a_0^2$	$0.390\pi a_0^2$	...	$0.322\pi a_0^2$
$1s2p_0$	$0.475\pi a_0^2$	$0.457\pi a_0^2$	$0.393\pi a_0^2$	$0.359\pi a_0^2$	...	$0.521\pi a_0^2$
$1s2p_T$	$1.04\pi a_0^2$	$1.21\pi a_0^2$	$0.87\pi a_0^2$	$1.14\pi a_0^2$	$0.92\pi a_0^2$	$1.17\pi a_0^2$

tions [actually four equations, since $\beta_{211}^{(1s)}(b, Z) = -\beta_{21-1}^{(1s)}(b, Z)$] is readily solved by elementary numerical techniques. Then, using Eq. (21), we may evaluate the various inelastic cross sections. We have done this for both e^- + H and e^+ + H for $k_i a_0 = 2(E_i \simeq 54$ eV), so we can compare with the results of Burke *et al.* at the highest energy in their calculation. The results are shown in Table I.

Before discussing the entries in Table I, we should point out that the exact e^- + H close-coupling results in column 3 of Table I were obtained with exchange included. However, the effects of exchange are probably quite negligible at $k_i a_0 = 2$, so our comparisons should be valid. For the e^+ + H system, no such difficulty arises since the Pauli exclusion principle plays no role in the e^+e^- wave function.

The most striking aspect of Table I is the discrepancy that exists between the Born results and the eikonal-Born results, where by the latter we mean the first nontrivial term in the iterative solution to Eq. (14) used in Eq. (21) for the total cross section. The differences are purely kinematical in origin since, for example, it is obvious that the same method applied to Eq. (17a) or Eq. (17b) would lead immediately to the usual Born results. [In these equations, the Born approximation consists simply in setting $\alpha_m^{(n)}(\vec{R}) = \delta_{nm}$.] A glance at Table I shows that these kinematical approximations leading from Eq. (17b) to Eq. (19) or (21) can easily have effects of the order of magnitude of 20%.

In order to make the most meaningful possible comparison, we therefore have returned to Eq. (17a) and used this to evaluate differential cross sections for the processes of interest. Actually, since the differences between the Born and close-coupling results are not too large, we have not evaluated Eq. (17a) exactly, but rather have evaluated the difference between Eq. (17a) and Eq. (19) in Born approximation. This is not as accurate as evaluating Eq. (17a) exactly, but since these few state methods are not our major concern, this approximation will suffice. The results are shown in Table II. We see that the changes from Table I are significant, but that, in general, the agreement is only qualitative between the two methods, especially if considered in terms of the difference between the Born approximation and the exact result. Note that in this case, since we start from Eq. (17a), the Born and eikonal-Born results agree exactly. It is interesting to note also that the eikonal results of Table II seem to be a bit better than the results that would be obtained by a straightforward time-dependent straight-line-trajectory approach. The results of such a method can be obtained directly from Table I by multiplying by $k_f/k_i = 0.9$. The qualitative improvements of Eq. (17a) over Eq. (19) make it a natural candidate for the further approximations which we shall make in Sec. IV.

IV. GLAUBER APPROXIMATION

We have already commented in the Introduction on the desirability of including a very large number of states in the close-coupled equations. We now

TABLE II. Comparison of eikonal- and exact-close-coupling results without kinematical simplifications.

Initial-final state	Born	Exact close coupling (e^- + H)	Modified eikonal close coupling (e^- + H)	Exact close coupling (e^+ + H)	Modified eikonal close coupling (e^+ + H)
$1s2s$	$0.102\pi a_0^2$	$0.101\pi a_0^2$	$0.098\pi a_0^2$	$0.138\pi a_0^2$	$0.185\pi a_0^2$
$1s2p_+$	$0.283\pi a_0^2$	$0.239\pi a_0^2$	$0.296\pi a_0^2$	...	$0.236\pi a_0^2$
$1s2p_0$	$0.475\pi a_0^2$	$0.393\pi a_0^2$	$0.367\pi a_0^2$	...	$0.524\pi a_0^2$
$1s2p_T$	$1.04\pi a_0^2$	$0.87\pi a_0^2$	$0.96\pi a_0^2$	$0.92\pi a_0^2$	$1.00\pi a_0^2$

show that, if we make use of Eq. (2), we can include an infinite number of states and obtain a closed form expression for $\alpha_{n'}^{(n)}(\vec{b}, Z)$. We begin by noting that according to Eq. (10)

$$q_{mn} Z \simeq a_0 \Delta / \hbar v_i ,$$

if we assume that important values of Z are of order a_0. We should remark that because of the long range of the Coulomb potential this assumption is somewhat shaky; clearly, for a nuclear potential with range a_0 this assumption would be quite reasonable. In the above equation Δ is a typical energy difference between important states of the composite system. Thus, using Eq. (2), we see that $q_{mn}Z$ is small compared to unity, so that

$$e^{i q_{mn} Z} \simeq 1 .$$

Using this result in Eq. (17) we find that

$$\mathfrak{U}_{mm'} = \mathfrak{V}_{mm'}$$

in the spirit of the Glauber approximation, so that Eq. (14) becomes

$$\frac{d\alpha_m^{(n)}(\vec{b}, Z)}{dZ} = -\frac{i\mathfrak{M}}{k_i a_0^2} \sum_{m'} \mathfrak{V}_{mm'}(b, Z) \alpha_{m'}^{(n)}(\vec{b}, Z) . \tag{14'}$$

If we let m' run over the complete set of internal states of the composite system, we can solve Eq. (14') exactly. Using closure, we can see immediately from Eq. (5) that

$$\alpha_m^{(n)}(b, Z) = \int d\vec{r}\ \phi_m^*(\vec{r})\, \phi_n(\vec{r}) \times \exp\left(-\frac{i\mathfrak{M}}{k_i a_0^2} \int_{-\infty}^{z} V(\vec{b}, Z', \vec{r})\, dZ' \right) . \tag{23}$$

Putting Eq. (23) into Eq. (19), we obtain for the scattering amplitude

$$T_{if} = \frac{k_i}{2\pi i} \int e^{i(\vec{k}_i - \vec{k}_f)\cdot\vec{b}} \phi_{n'}^*(\vec{r})\, \phi_n(\vec{r}) \times \left[\exp\left(\frac{i\mathfrak{M}}{k_i a_0^2} \int_{-\infty}^{\infty} V(\vec{b}, Z, \vec{r})\, dZ \right) - 1 \right] d\vec{b}\, d\vec{r} , \tag{24}$$

where the symbols are as defined above.

Equation (24) has two features which are very undesirable. First, because the minimum value of $\vec{k}_i' - \vec{k}_f$ is zero, it can be shown that the total cross section for an "optically-allowed" transition is infinite.[8] This is obvious if one looks at the first nonvanishing contribution from the expansion of the eikonal exponential. Although this is consistent with unitarity in the sense that the imaginary part of the elastic amplitude is infinite in the forward direction, it is very unsatisfactory from a practical point of view. This infinity results from the long range of the Coulomb potential and would not occur in problems involving nuclear potentials, where Eq. (24) could be used with confidence if Eqs. (1a), (1b), and (2) were satisfied. A second, more detailed, feature of Eq. (24) which is rather unfortunate is that it predicts that for s-p transitions in e + H collisions transitions to the $m = 0$ substate of the p state are strictly forbidden.

It seems to us that the most natural way to remedy these difficulties is as follows. Looking back at Eq. (17a), let us set $e^{-iq_{mn}Z} \simeq 1$ in that equation. If we now insert Eq. (23) for $\alpha_m^{(n)}(\vec{R})$ into Eq. (17a) the sum can be done by closure, leaving us with

$$T_{if} = -\frac{\mathfrak{M}}{2\pi a_0^2} \int e^{i(\vec{k}_i - \vec{k}_f)\cdot\vec{R}}\ \phi_{n'}^*(\vec{r})\, \phi_n(\vec{r})\, \mathfrak{V}(\vec{b}, Z, \vec{r}) \times \exp\left(-\frac{i\mathfrak{M}}{k_i a_0^2} \int_{-\infty}^{Z} V(\vec{b}, Z', \vec{r})\, dZ' \right) d\vec{b}\, dZ\, d\vec{r} . \tag{25}$$

This expression, although it has been obtained through somewhat *ad hoc* procedures, has the advantages of possessing correct kinematics and also retaining the key feature of Eq. (24), namely, the eikonal exponential oscillates when the incident electron is near one of the bound electrons in the target. We shall refer to Eq. (25) as the Glauber approximation.[9] The presence of the correct momentum transfer in Eq. (25) insures that the large-R part of the integral will be cut off properly and there will be no infinite cross sections appearing in the theory, although the elastic amplitude is still weakly divergent in the forward direction. We should note that because of the simplicity of the Coulomb potential the eikonal phase can be evaluated exactly for anv atom using the fact that

$$\int_{-\infty}^{z_2} \left(\frac{1}{|\vec{r}_2 - \vec{r}_1|} - \frac{1}{r_2} \right) dz_2 = \ln \left(\frac{r_2 - z_2}{|\vec{r}_2 - \vec{r}_1| - z_2 + z_1} \right) .$$

The problems involved in the evaluation of Eq. (25) are formidable. Even for the simple e + H case, Eq. (25) involves a six-dimensional integration, whereas Eq. (24) can be reduced to a relatively uncomplicated two-dimensional integral involving only simple transcendental functions. This integral can be done numerically with ease. Unless some further undesirable approximations are made concerning the momentum transfer Eq. (25) cannot be simplified.

Fortunately, the recent generations of high-speed computing machines have made it possible to do integrals like the one in Eq. (25) by brute force, We have elected to do the integration by the Monte Carlo method which consists essentially in evaluating the integral at a large number of points chosen randomly in the multidimensional integration space. The sum of these values divided by the number of points gives an approximation to the integral which improves as the number of points is increased. Actually, since a few of the variables are integrated

over an infinite range, it is convenient to pick some of the variables with respect to a weight function which is determined essentially by the bound-state wave functions. The integral over the radial coordinate of the incident electron is slowly convergent, so it was done by integrating on this variable out to some large, finite distance using the Monte Carlo method and then doing the rest of the integral by expanding the eikonal phase and keeping only the lowest-order contribution, which can, in fact, be evaluated exactly. This is equivalent to using Born-approximation phase shifts for large angular momenta. The eikonal phase was retained out to $r_{in} = 20$ a.u., where r_{in} is the radial coordinate of the incident electron. Checks performed by keeping the eikonal phase out to $r_{in} = 30$ a.u. agreed with the results obtained by keeping the eikonal phase out to $r_{in} = 20$ a.u., to within statistical errors.

An excellent check on the accuracy of the Monte Carlo method itself is provided by doing the Born-approximation integrals by this technique. Since the Born integrals can be done in terms of simple functions for systems such as $e + H$ and $e + He$, one can check the accuracy of the procedure. A particular advantage of this method is that for atoms other than hydrogen, the fact that the target-atom wave functions are very complicated offers no significant difficulties.

V. DISCUSSION AND RESULTS

A. Electron-Helium Scattering

In order to test the Glauber approximation, let us first look at the process $e^- + He$. This is particularly well suited for experimental investigation because the target gas is inert, and at the same time the target-gas wave functions are sufficiently simple to make accurate calculations possible. Recent experiments by the Electron Physics Group at the National Bureau of Standards[10,11] have culminated in an absolute measurement of $e^- + He$ differential cross sections at 5° for a number of processes.[11] We will concentrate on $e^- + He(1s^2) \rightarrow e^- + He(1s2p\,^1P_1)$ in what follows. These absolute measurements, carried out at several different energies, calibrate earlier relative measurements of differential cross sections by the N. B. S. group.[10] We then fit the differential cross-section values obtained at various angles to the simple analytic form (see Ref. 10, where a similar form is used):

$$\frac{d\sigma}{d\Omega} = \frac{A}{\Delta^2(a^2+\Delta^2)^6} + \frac{B}{(a^2+\Delta^2)^7}\,, \tag{26}$$

where $\Delta^2 = k_i^2 - k_f^2 - 2k_i k_f \cos\theta$. Integrating Eq. (26) over all angles one finds total cross sections for the $1\,^1S_0 \rightarrow 2\,^1P_1$ transition in reasonable agreement with optical measurements.

We have evaluated the $1\,^1S_0 \rightarrow 2\,^1P_1$ scattering amplitude by using Eq. (25) along with the familiar six-parameter Hylerras[12] wave function for the ground state and an Eckart[13] screened hydrogenic wave function for the excited state ("inner charge" equal to 2.003, "outer charge" equal to 0.965).[14] We used 100 000 randomly chosen points in the nine-dimensional space for the Monte Carlo integrations at each value of the momentum transfer. A typical result (for $E_i = 103$ eV) is shown in Fig. 1. For comparison, the dashed curve shows our fit to the experimental results of CMK at 100 eV using Eq. (26). The fit is seen to be excellent.

Before attempting to compare experiment with theory, several comments should be made on the reliability of the Monte Carlo method. From Fig. 1, it is clear that statistical fluctuations at a given momentum transfer are significant. On the other hand, one might expect that in integrating over all angles to obtain total cross sections the effect of such fluctuations would be reduced, since there is no correlation between errors in $d\sigma/d\Omega$ at different values of the momentum transfer. Thus, the total cross sections are undoubtedly more reliable than any particular value of $d\sigma/d\Omega$ at some momentum transfer. Since we evaluate both the Born and the Glauber differential cross sections by Monte Carlo

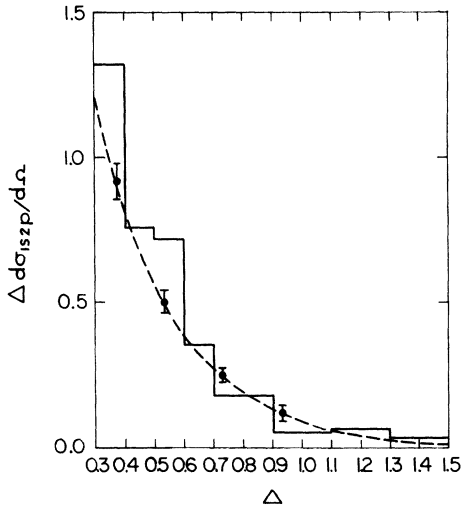

FIG. 1. Differential cross section for excitation of the $1s2p\,^1P$ state of helium by electron bombardment as a function of momentum transfer Δ; the incident electron energy is 100 eV and the minimum physically allowed value of Δ is Δ = 0.305. Differential cross section is multiplied by Δ for convenience of scale. The dashed curve is a fit using Eq. (26) to the results of Ref. 10 as normalized by Ref. 11; the dots are experimental points (with experimental uncertainties as shown) at 5°, 10°, 15°, and 20°. The solid curve represents the results of the eikonal approximation in which Eq. (25) is evaluated at a number of values of Δ by the Monte Carlo method. All quantities are in atomic units.

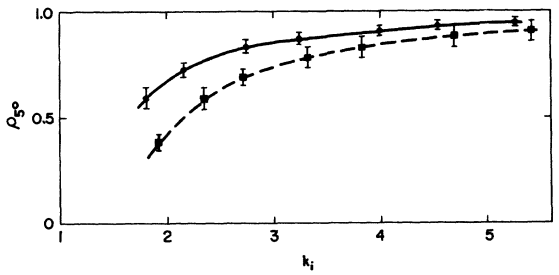

FIG. 2. Ratio of the Born differential cross section at 5° [for $e^- + \mathrm{He}\ (1s^2) \rightarrow e^- + \mathrm{He}\ (1s2p\ ^1P)$] to the eikonal differential cross section at 5° for the same process is shown in the solid curve. The dashed curve is the ratio of the Born differential cross section as measured in Ref. 11. k_i is the incident electron momentum in atomic units. The error bars on the solid curve represent statistical uncertainties in performing the Monte Carlo integrations. The error bars on the dashed curve represent experimental errors.

methods, it might be hoped that the ratio of these two quantities would be more accurate than either one individually. That this is indeed the case was verified by computing the ratio

$$\rho_\theta = \left(\frac{d\sigma(\theta)}{d\Omega}\right)_{\mathrm{eik}} \Big/ \left(\frac{d\sigma(\theta)}{d\Omega}\right)_{\mathrm{Born}}$$

at a fixed angle and doing such a computation several times (always using 100 000 random points in each computation). The statistical spread between independent evaluations of the ratio was quite small, and we feel that ρ_θ is the most accurately determined quantity.

Figures 2 and 3 show ρ_{5° and ρ_{10° compared with the measurements of CMK and of Ref. 10 as normalized by the results of CMK. The error bars on the theoretical curve represent the results of a statistical analysis of several determinations of ρ. As one would expect, the results at low energy, particularly for ρ_{5°, reveal a strong disagreement between experiment and theory, with the agreement improving at higher energies. The most striking aspect of Figs. 2 and 3 is the fact that even at $k_i \simeq 5$ ($E_i \cong 400$ eV) one sees experimentally that there is a significant departure from the Born approximation at both 5° and 10° and that the Glauber approximation also shows such a behavior.

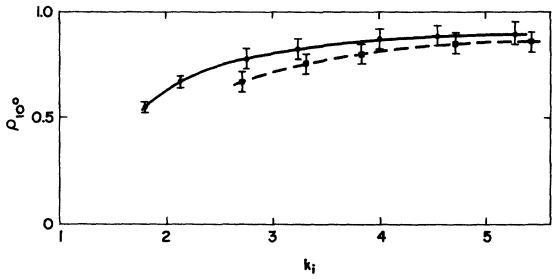

FIG. 3. Ratio of the Born differential cross section at 10° [for $e^- + \mathrm{He}\ (1s^2) \rightarrow e^- + \mathrm{He}\ (1s2p\ ^1P)$] to the eikonal differential cross section at 10° for the same process is shown in the solid curve. The dashed curve is the ratio of the Born differential cross section at 10° to the corresponding experimental differential cross section as measured in Ref. 10 and normalized by Ref. 11. k_i is the incident momentum in atomic units. The error bars on the solid curve represent statistical uncertainties in performing the Monte Carlo integrations. The error bars on the dashed curve represent experimental errors.

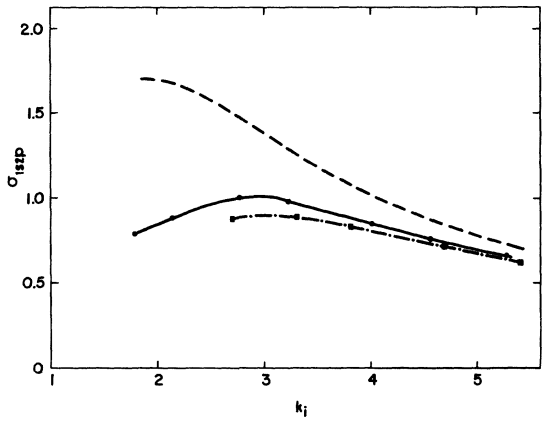

FIG. 4. Total cross section for the excitation of the $1s2p\ ^1P$ state of helium by electron bombardment as a function of k_i, the incident electron momentum. σ_{1s2p} is in units of πa_0^2; k_i is in atomic units. The upper curve is the Born approximation; the middle curve represents the results of this paper using Eq. (25); and the bottom curve shows the results of Ref. 10 (normalized at 5° by Ref. 11). The differential results of Ref. 10 were turned into total cross sections by fitting them to Eq. (26).

Finally, in Fig. 4, we show the total integrated cross section for the process in question. The departure at low energy from the Born approximation is striking, as is the agreement between experiment and theory. This comparison is less compelling than the ones presented in Figs. 2 and 3 since the "experimental" curve involves an extrapolation via Eq. (26) and the theoretical curve is less precise than the theoretical curves in Figs. 2 and 3.

On the basis of a few spot checks involving two independent measurements of $d\sigma/d\Omega$ at a fixed energy and over a complete range of momentum transfers, we feel that the error in the theoretical curve is of the order of 10%. In fact, as far as the Born approximation is concerned, our values of the total Born cross section obtained by the Monte Carlo method agreed at all energies to within 6% with the exact result. Of course, the amplitude integral of Eq. (25) has more oscillation in it than does the corresponding Born amplitude integral as a result

of the eikonal phase. Thus, in a statistical integration, the Glauber results cannot be expected to be quite as accurate as the Born results.

If at each momentum transfer studied one used the same methods that were employed in obtaining ρ_{5° and ρ_{10° (namely, repeated evaluation of $d\sigma/d\Omega$, followed by statistical averaging), then, of course, one could give a better estimate of the "theoretical error" in Fig. 4. However, the amount of computer time involved in this more precise attack seemed extravagant. At this point, it would appear that a more important task is to obtain a better understanding of why the agreement between experiment and theory is as good as it is.

B. Electron-Hydrogen Scattering

The situation in $e^- + H$ scattering is qualitatively similar to that found in the case of $e^- + He$, but here we have the additional possibility of looking at results on the polarization of the radiation emitted from the final state of the scattering process $e^- + H(1s) \rightarrow e^- + H(2p)$. Such information is not available in the case discussed above involving the 2^1P_1 state of helium since the 584-Å line in question is extremely difficult to deal with experimentally. However, the 1216-Å ($2p \rightarrow 1s$) line in hydrogen is accessible to experiment and has been studied by Ott *et al.* [15] In these experiments, the $2p$ state is produced via the reaction $e^- + H(1s) \rightarrow e^- + H(2p)$. The relative population of magnetic sublevels gives rise to a polarization of the emitted radiation. This polarization is a very important quantity since in the modified eikonal result of Eq. (24), the polarization is independent of energy and equal to $-\frac{3}{11}$. The polarization for this case is given to sufficient accuracy by

$$P = 3(1-x)/(7+11x) ,$$

where $x = \sigma_+/\sigma_0$, σ_+ being the cross section for $e^- + H(1s) \rightarrow e^- + H(2p_+)$ and σ_0 being the cross section for $e^- + H(1s) \rightarrow e^- + H(2p_0)$.

For the case of a hydrogen target, we followed the same procedure as discussed above for helium, except that the *exact* bound-state wave functions of hydrogen could be used in Eq. (25) for both the initial and final states of the target. The integration is over a six-dimensional space and was done by the Monte Carlo method, again using 100 000 randomly chosen points. We looked at both the $2s$ and $2p$ final states. Several workers[2,5] have already investigated this problem under the dynamically undesirable assumption that the momentum transfer is perpendicular to the incident momentum, as mentioned above in relation to Eq. (24) this gives a selection rule $\Delta m = \pm 1$ for $s \rightarrow p$ transitions, leading to a polarization

$$P = -\tfrac{3}{11} .$$

This result is in strong disagreement with experiment; the work of Ott *et al.* [15] shows that P is positive from threshold to about 250 eV.

Such a serious discrepancy is perhaps not surprising given the drastic nature of the assumption that the angle between the incident direction and the momentum transfer is 90°. In fact, for forward scattering this angle is always 0°. When $k_i = 1.5$, the largest value the angle attains is only about 55°; when $k_i = 2.0$, the largest value the angle attains is about 65°.

To begin with, we shall discuss briefly the $1s$-$2s$ excitation process. Our result for σ_{1s2s} as a function of k_i agree virtually exactly with the calculations of Refs. 2 and 5 which made essential use of the assumption

$$\vec{\Delta} \perp \vec{k}_i . \tag{27}$$

Taking cascade from higher p states into account, Tai *et al.* [5] find good agreement between experiment and theory and a very significant improvement over both close-coupling calculations and the Born approximation which, in the energy range considered ($k_i \gtrsim 1.5$), are very nearly equal. Since our results are identical with those obtained under the assumption of Eq. (27) (which have been very thoroughly discussed by Tai *et al.*), we shall not comment further on them here; we will have more to say about this case in relation to positron-hydrogen scattering (Sec. VC).

The $1s$-$2p$ process contains more interesting information. Our results are summarized in Figs. 5 and 6. Figure 5 shows the polarization P as a function of k_i. The results of our calculation, given by the solid line, fall systematically below the experimental points of Fite *et al.*, although there is obviously a major improvement over the result $P = -\frac{3}{11}$ obtained using the assumption of Eq. (27). The error bars are a rough estimate of our Monte Carlo

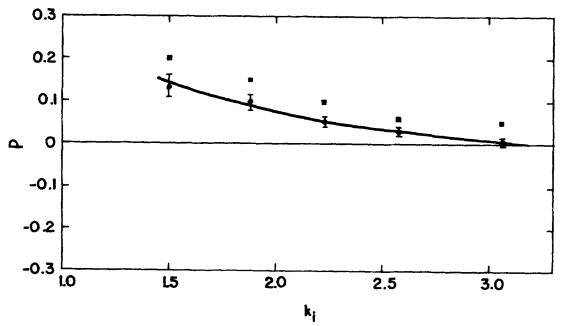

FIG. 5. Polarization P of reemitted radiation following electron excitation of the $2p$ state of atomic hydrogen as a function of the incident electron momentum k_i in atomic units. The solid curve represents the results of this paper; the squares represent the experimental results of Ref. 15.

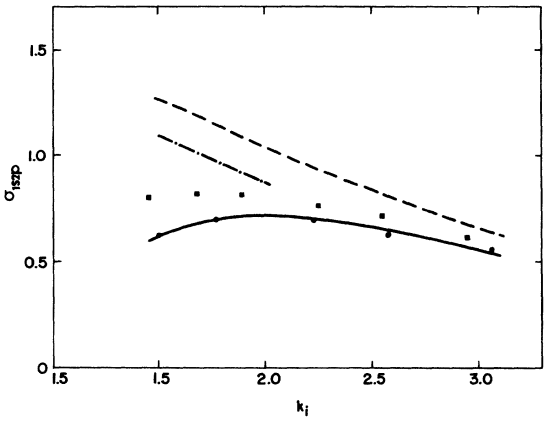

FIG. 6. Total cross section (in units of πa_0^2) for the excitation of the $2p$ state of atomic hydrogen by electron bombardment as a function of the incident electron momentum k_i in atomic units. The upper curve is the Born approximation; the second curve is the five-state close-coupling calculation of Ref. 6; and the bottom curve is the result of this paper using Eq. (25). The solid squares are the experimental results of Ref. 16.

error in P, which was found to be significantly more sensitive to random error than σ_{1s2p}. Figure 6 shows σ_{1s2p} as a function of k_i. Included for comparison are the five-state close-coupling result of Burke, Schey, and Smith[6] and the Born-approximation curve. The theoretical curve, which we feel represents the content of Eq. (25) to better than 10%, lies a bit below the experimental results,[16] but represents a substantial improvement over the Born approximation. We may conclude, as in the case of helium, that Eq. (25) gives a good qualitative explanation of experimental results and a reasonable account of departures from the Born approximation.

C. Positron-Hydrogen Scattering

The case of positron-hydrogen scattering (or, equivalently, proton-hydrogen scattering) is of interest because of the fact that both the Born approximation and the results of Refs. 2 and 5 [which make use of the assumption of Eq. (27)] predict that e^+-H scattering cross sections and e^--H scattering cross sections should be identical, whereas the close-coupling method shows very significant differences between the two cases. The differences between positron scattering and electron scattering in the close-coupling approach are particularly pronounced in the case of the excitation of the $2s$ state of hydrogen, so we have examined this case using Eq. (25). The results are shown in Fig. 7. The upper curve shows the steeply rising Born curve which is the same for both electron and positron excitation of the $2s$ state. The solid curve shows the results for electron excitation using Eq. (25); as remarked above this curve, when corrected for cascade, agrees well with experiment. The remaining curve shows the results for positron excitation, we see that the differences between positron and electron excitation are particularly striking below an incident momentum of about 2 a.u. This illustrates once again the importance of treating the kinematics of the momentum transfer correctly. It would be extremely interesting to have experimental evidence pertaining to this question; since positron scattering is not feasible, proton scattering from hydrogen in the range 50–150 keV would be desirable. Since the results for proton excitation scale quite well with the velocity in the velocity range shown, the results for $p + \mathrm{H}(1s) \rightarrow p + \mathrm{H}(2s)$ will be very similar to the positron results of Fig. 7. For example, even at the lowest velocity shown in Fig. 7, the value of the cross section by proton excitation will be only about 5% above the value for positron excitation. Proton-hydrogen excitation would have the additional interest that the assumptions of Eqs. (1a) and (1b) are very well satisfied, so one would have a direct test of Eq. (2).

VI. CONCLUSIONS

We have tried to give a discussion of the eikonal approximation which relates it clearly to the commonly used close-coupling method and have attempted to isolate the key assumptions and test them by comparison with exact calculations and with experiment. On the basis of this work we can say that the eikonal method has qualitatively very satisfactory behavior: In both e-He scattering and

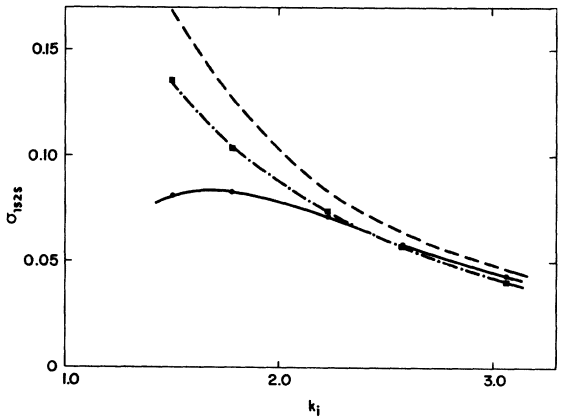

FIG. 7. Cross sections (in units of πa_0^2) for the excitation of the $2s$ state of atomic hydrogen by electron and positron bombardment as a function of the incident projectile momentum k_i in atomic units. The upper curve is the Born approximation result which is the same for electrons and positrons; the solid curve is the result for electron bombardment computed using Eq. (25); and the remaining curve is the result for positron bombardment computed using Eq. (25).

e-H scattering reasonable (although not perfect) agreement is found between theory and experiment. It is clear that in atomic physics applications it is necessary to treat the momentum transfer in as correct a manner as possible; in order to do this we have utilized the Monte Carlo method to deal with integrals which would otherwise necessitate serious kinematical approximations. This has the additional advantage of enabling us to tackle problems with more complicated wave functions than simple hydrogenic ones. In particular, for the excitation of helium, where good wave functions are mandatory, we have been able to extract the exact consequences of the eikonal hypothesis and test them against what are probably the most accurate electron scattering experiments available.

Obviously the above methods could be routinely applied to other transitions, and it may even be possible to give a much improved account of exchange scattering using these eikonal Monte Carlo techniques, although serious difficulties must be overcome.[17] Perhaps the first order of business, however, would be to do a more precise job on the Monte Carlo integrations using a present generation computer which, because of its great speed, would enable one to use many more random integration points and thereby reduce our "theoretical error bars."

One particularly interesting question remains for direct collisions, namely, the excitation of atomic hydrogen by proton impact. If such experiments can be done in the 50–150-keV range, we predict that one will find (at the same velocity) a very significant difference between $p + \mathrm{H}(1s) \rightarrow p + \mathrm{H}(2s)$ and $e^- + \mathrm{H}(1s) \rightarrow e^- + \mathrm{H}(2s)$.

ACKNOWLEDGMENTS

Eikonal results using the assumption of Eq. (27) were obtained for several of the processes discussed in this paper while the author was a visitor at the Université Libre de Bruxelles. The author gratefully acknowledges the support of the Alfred P. Sloan Foundation which made this visit possible and the hospitality of Professor M. Demeur and C. J. Joachain. The results reported in this paper were obtained with the aid of the University of Massachusetts CDC 3600 computer. The author thanks the University of Massachusetts for a Computer Research Grant. Finally, the author thanks Professor W. J. Mullin for explaining to him the power of the Monte Carlo method.

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[7]See, for example, Ref. 1, p. 341.

[8]Strictly speaking [see following Eq. (17b)], the quantity $|\vec{k}_i' - \vec{k}_f|$ is not zero at $\theta = 0$, but is rather of order $1/k_i^3$. Thus, for example, the total cross section for the excitation of the $2p$ state of atomic hydrogen would never tend to the Born-approximation result, no matter how high the incident energy, remaining always larger than the Born cross section.

[9]This result was first obtained by Glauber in Ref. 1. We have "derived" it here in a different manner which we hope is more illuminating for atomic physics.

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[14]These wave functions are by no means the most accurate ones available. However, at least for the Born approximation, they lead to results which differ only by a few percent from those obtained using high-precision helium wave functions. See, for example, Y. K. Kim and M. Inokuti, Phys. Rev. 175, 176 (1968).

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

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[17]The author has actually used these Monte Carlo methods in conjunction with the eikonal approximation to investigate exchange contributions to the process $e^- + \mathrm{H}(1s) \rightarrow e^- + \mathrm{H}(2s)$ in the vicinity of $k_i = 1$. The results obtained, when combined with nonexchange contributions, agree very well with the experiment of W. L. Lichten and S. Schultz [Phys. Rev. 116, 1132 (1959)] but disagree with the experiment of W. L. Fite *et al.* [Phys. Rev. 116, 356 (1959)]. Since Fite *et al.* go up to rather high energy and normalize to the Born approximation, their results are presumably to be preferred to those of Lichten and Schultz which are normalized to the Born approximation at 45 eV. In fact, if one renormalizes the results of Lichten and Schultz (at, say, 45 eV) to those of Fite *et al.*, the two agree rather well. Of course, the use of eikonal-scattering wave functions at $k_i = 1$ is surely very suspect, so the results obtained for the exchange contribution (and the direct contribution also) are probably not reliable.