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Glauber Theory of Atomic-Hydrogen Excitation by Electron Impact*

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The Glauber approximation has been applied to excitation of the $2s$, $2p$, $3s$, and $3p$ levels of the hydrogen atom by electron impact. The differential and integrated excitation cross sections predicted by the Glauber theory have been compared with experiment and with other calculations. The Glauber approximation is a considerable improvement over the Born approximation at energies $<\sim 100$ eV. At energies $>\sim 100$ eV, the Glauber total excitation cross sections approach the Born approximation, even though at large scattering angles ($>40°$) the Glauber differential cross sections may be very different from the Born approximation. At intermediate energies (~ 30–100 eV), the Glauber predictions are surprisingly good; at energies $<\sim 20$ eV, the Glauber integrated cross sections are smaller than those observed experimentally.

I. INTRODUCTION

In the past, the Glauber[1] approximation for scattering amplitudes was applied to many problems in particle physics and in nuclear physics.[2] More recently, the Glauber approximation was employed in the elastic scattering of electrons by hydrogen atoms.[3,4] In these latter calculations – for angular distributions as well as for total elastic cross sections – the Glauber theory agrees surprisingly well with experiment, even at comparatively low electron energies ($<\sim 100$ eV), where Glauber's formulation might be expected to break down. As a matter of fact, Glauber's theory is essentially a diffraction approximation[5] wherein it is assumed that the incident plane wave sweeps virtually undeviated through the region of interaction and emerges suffering only a position-dependent change of phase and amplitude; obviously this assumption is likely to be invalid at low energies. On the other hand, the Glauber theory has the virtue – to which its aforementioned success in e-H elastic scattering perhaps can be ascribed – that it takes account of the interactions of the incident electron with both the target electron and the target proton; for excitation processes, in most other easily computed approximations, the interaction between the incident electron and the proton either produces identically zero scattering [first Born approximation (FBA)], or else is assumed to produce negligible scattering (impulse approximation,[6] Vainshtein approximation[7]).

In view of the preceding, it seems reasonable to examine the utility of Glauber theory in the inelastic scattering of atomic hydrogen by electrons, especially at energies <100 eV, where the FBA is known to be very poor (see Sec. IV). The specific reactions examined by us include excitation of H($1s$) to the $2s$, $2p$, $3s$, and $3p$ levels. The derivations of the theoretical formulas employed are given in Secs. II and III. Sections IV and V discuss the results obtained, including their comparison with experiment.

II. BASIC FORMULAS

In what follows we suppose the target proton to be infinitely heavy. Also, we neglect exchange scattering, which is not readily estimated in a diffraction theory like Glauber's; the possible significance of this neglect will be discussed in Sec. V. Let $\hbar\vec{K}_i$, $\hbar\vec{K}_f \equiv m\vec{v}_i$, $m\vec{v}_f$ be, respectively, the momentum vectors of the incident electron before and after the collision, and define

$$\vec{q} = \vec{K}_i - \vec{K}_f \, .$$

We place the origin of coordinates at the proton, with the z axis (also the polar axis) along $\vec{K}_i$. Let $\vec{r}, \vec{r}\,'$ denote, respectively, the position vectors of the target and incident electrons, and write $\vec{r} = \vec{s} + \vec{z}$, $\vec{r}\,' = \vec{b} + \vec{\zeta}$, where (see Fig. 1) $\vec{s}$ is the projection of $\vec{r}$ onto the x, y plane; correspondingly, the impact parameter vector $\vec{b}$ lies in the x, y plane and is the perpendicular from the origin to the incident particle's initial trajectory.

With these definitions, the amplitude $F_{fi}(\vec{q})$ for collisions in which the atom undergoes a transition from an initial state i with wave function u_i to a

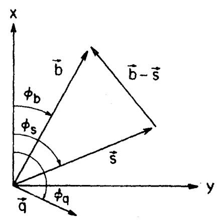

FIG. 1. Projection of the collision on the x, y plane. The x, y plane is the plane of the paper; the initial velocity of the incident electron coincides with the direction of positive z, which is into the paper. The vectors $\vec{b}$, $\vec{s}$, and $\vec{q}$ lie in the x, y plane, and have azimuth angles ϕ_b, ϕ_s, ϕ_q, respectively, measured from positive x, as shown.

final state f with wave function u_f, and in which the incident particle imparts a momentum $\hbar\vec{q}$ to the target is given by[1]

$$F_{fi}(\vec{q}) = \frac{iK_i}{2\pi}\int u_f^*(\vec{r})\,\Gamma(\vec{b},\vec{r})\,u_i(\vec{r})\;e^{i\vec{q}\cdot\vec{b}}\,d^2b\,d\vec{r}\,, \qquad (1)$$

where it has been assumed that the vector $\vec{q}$ is perpendicular to $\vec{K}_i$, i.e., that $\vec{q}$ also lies in the x, y plane (Fig. 1). This assumption is specifically employed in the reduction of Eq. (1) to usable form (see Sec. III); its significance is discussed below, mainly in Sec. IV. Moreover, in Eq. (1)

$$\Gamma(\vec{b},\vec{r}) = 1 - e^{i\chi(\vec{b},\vec{s})}\,, \qquad (2)$$

where the phase-shift function

$$\chi(\vec{b},\vec{s}) = -(1/\hbar v_i)\int_{-\infty}^{\infty} V(\vec{b},\vec{r},\zeta)\,d\zeta$$

is the integral – along the trajectory of the incident electron – of the instantaneous potential between the incident particle and the target. For electrons incident on atomic hydrogen, we find readily[3]

$$\chi(\vec{b},\vec{s}) = 2n\ln(|\vec{b}-\vec{s}|/b)\,, \qquad (3)$$

where $n = e^2/\hbar v_i$.

When the exponential in (2) is expanded in powers of χ, the first nonvanishing term in (1) is linear in χ, and can be seen to be identical with the FBA. Retention of only the linear terms in χ should be valid at large v_i. Thus, one might infer that the Glauber predictions for $F_{fi}(\vec{q})$ should merge with the FBA at sufficiently high incident energies. This inference is not really justified, however, for reasons which will be discussed in Sec. IV below. In particular, for the inelastic cross sections examined in this paper, the Glauber and the FBA predictions at large scattering angles (~60°, for instance) apparently do not approach each other as the incident energy is increased. However, at high energies, large-angle scattering generally makes a relatively inconsequential contribution to integrated cross sections, whether elastic or inelastic. Therefore we do expect that the Glauber total (i.e., integrated over angle) inelastic cross sections will approach the FBA at sufficiently high energies. For the excitation processes examined in this paper, the Glauber total cross sections become essentially indistinguishable from the FBA at incident energies E_i > 200 eV.

In excitation from state i to state f, the differential cross section is

$$\frac{d\sigma_{fi}}{d\Omega} = \frac{K_f}{K_i}\,|F_{fi}(\vec{q})|^2\,, \qquad (4)$$

and the total cross section is

$$\sigma_{fi} = \int (K_f/K_i)\,|F_{fi}(\vec{q})|^2 \sin\theta\,d\theta\,d\phi\,, \qquad (5)$$

where θ, ϕ are the angles in spherical coordinates specifying the direction of $\vec{K}_f$ relative to $\vec{K}_i$. Even in e–H (1s) collisions, the quantity $F_{fi}(\vec{q})$ need not be independent of ϕ, i.e., need not be axially symmetric about the z axis when u_f denotes a final state of specified magnetic quantum number, e.g., in the 1s-2p excitation of hydrogen; of course, the differential cross section summed over final magnetic quantum numbers is independent of ϕ.

The quantity K_f is fixed by

$$(\hbar^2/2m)K_f^2 + \epsilon_f = (\hbar^2/2m)K_i^2 + \epsilon_i\,, \qquad (6a)$$

where ϵ_i, ϵ_f are the energies of the initial and final atomic states (with $\epsilon_i = -13.6$ eV in the reactions we discuss). Thus from

$$q^2 = K_i^2 + K_f^2 - 2K_iK_f\cos\theta, \qquad q\,dq = K_iK_f\sin\theta\,d\theta\,, \qquad (6b)$$

we can recast Eq. (5) into the form

$$\sigma_{fi} = (1/K_i^2)\int_{K_i-K_f}^{K_i+K_f} dq\,q\int_0^{2\pi} d\phi\,\left|F_{fi}(\vec{q})\right|^2. \qquad (7)$$

III. CROSS-SECTION EXPRESSIONS

The desired expressions for inelastic 1s-2s, 1s-2p, 1s-3s, and 1s-3p excitation of atomic hydrogen by electrons now can be obtained from Eqs. (1), (4), and (7), along with the appropriate initial and final wave functions. Section III A details the reduction of the integral [(1)] to usable form in the 1s-2s case. As will be seen, the analysis closely parallels the previously reported[3] reduction of (1) in elastic e-H scattering.

A. 1s-2s Excitation

Introducing atomic units, for the 1s-2s excitation

$$F_{fi}(\vec{q}) = \frac{iK_i}{2\pi}\int \frac{1}{4\pi\sqrt{2}}\,(2-r)\,e^{-3r/2}\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2in}\right]$$

$$\times\, e^{i\vec{q}\cdot\vec{b}}(b\,db\,d\phi_b)(s\,ds\,d\phi_s\,dz)\,, \qquad (8)$$

where, because $\vec{q}$ is assumed to lie in the x, y plane containing $\vec{b}$ and $\vec{s}$ (see Fig. 1),

$$\begin{aligned} q\cdot b &= q\,b\cos(\phi_b-\phi_q)\,, \\ |\vec{b}-\vec{s}| &= [b^2+s^2-2bs\cos(\phi_s-\phi_b)]^{1/2} \end{aligned} \tag{9}$$

and of course $r=(s^2+z^2)^{1/2}$. Moreover, for a given $\vec{K}_f$, i.e., for a given direction of scattering specified by given θ, ϕ in Eq. (5), then as we have defined $\vec{q}$, we obtain $\phi_q=\phi+\pi$. Expression (8) can be rewritten in the form

$$F_{fi}(\vec{q}) = \left[\left(2+\frac{\partial}{\partial\lambda}\right)I_1(\vec{q},\lambda)\right]_{\lambda=3/2} \tag{10}$$

$$I_1(\vec{q},\lambda) = \frac{iK_i}{8\pi^2\sqrt{2}}\int e^{-\lambda r}\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2in}\right] \times e^{i\vec{q}\cdot\vec{b}}(bdb\,d\phi_b)(sds\,d\phi_s dz)\,. \tag{11}$$

Using (9) and $Y=2bs/(b^2+s^2)$, we obtain

$$I_1 = \frac{iK_i}{8\pi^2\sqrt{2}}\int e^{-\lambda r}\left[2\pi-\left(\frac{2s}{bY}\right)^{in}\int_0^{2\pi}d\phi_s(1-Y\cos\phi_s)^{in}\right] \times e^{i\vec{q}\cdot\vec{b}}(bdb\,d\phi_b)(sds\,dz)\,, \tag{12}$$

$$I_1 = \frac{iK_i}{4\pi\sqrt{2}}\int_0^\infty db\int_0^\infty ds\int_{-\infty}^\infty dz\,bs\,e^{-\lambda(s^2+z^2)^{1/2}}J_0(qb) \times\left[2\pi-\left(\frac{2s}{bY}\right)^{in}\int_0^{2\pi}d\phi_s(1-Y\cos\phi_s)^{in}\right], \tag{13}$$

$$I_1 = \frac{iK_i}{2\pi\sqrt{2}}\int_0^\infty db\int_0^\infty ds\,s^2bK_1(\lambda s)J_0(qb) \times\left[2\pi-\left(\frac{2s}{bY}\right)^{in}\int_0^{2\pi}d\phi_s(1-Y\cos\phi_s)^{in}\right]. \tag{14}$$

The result (14) is obtained from (13), e.g., by introducing the new integration variable τ instead of z via $z=s\sinh\tau$, and then employing a standard formula[8] for K_ν, the modified Bessel function of the third kind.

The integral (14) is further reduced by transforming to polar coordinates in the b, s plane,

$$s=R\sin\theta',\quad b=R\cos\theta'$$

This transformation makes Y and s/bY in (14) independent of R, so that we can use[9]

$$\int_0^\infty dR\,R^4K_1(\lambda R\sin\theta')J_0(qR\cos\theta') = [2^4/(\lambda\sin\theta')^5]\;{}_2F_1(3,2;1;-(q^2/\lambda^2)\cot^2\theta')\,. \tag{15}$$

Furthermore,[10]

$$\begin{aligned} {}_2F_1[3,2;1;-(q^2/\lambda^2)\cot^2\theta'] &= [1+(q^2/\lambda^2)\cot^2\theta']^{-4}\;{}_2F_1[-2,-1;1;-(q^2/\lambda^2)\cot^2\theta'] \\ &= [1+(q^2/\lambda^2)\cot^2\theta']^{-4}[1-(2q^2/\lambda^2)\cot^2\theta']\,. \end{aligned} \tag{16}$$

Therefore,

$$I_1 = \frac{16iK_i}{\sqrt{2}}\int_0^{\pi/2}\frac{d\theta'\sin^2\theta'\cos\theta'}{(\lambda\sin\theta')^5} \times\left(1+\frac{q^2}{\lambda^2}\cot^2\theta'\right)^{-4}\left(1-\frac{2q^2}{\lambda^2}\cot^2\theta'\right) \times\left[1-\frac{1}{2\pi}\left(\frac{1}{\cos\theta'}\right)^{2in}\int_0^{2\pi}d\phi_s(1-\sin2\theta'\cos\phi_s)^{in}\right]. \tag{17}$$

From Eqs. (10) and (17), after setting $\lambda=\frac{3}{2}$, we obtain

$$F_{fi}(\vec{q}) = \frac{2^{10}iK_i}{3^6\sqrt{2}}\int_0^{\pi/2}d\theta'\frac{\sin^3\theta'\cos\theta'}{(\sin^2\theta'+\frac{4}{9}q^2\cos^2\theta')^5} \times\left\{[-2\sin^4\theta'+\tfrac{56}{9}q^2\cos^2\theta'\sin^2\theta'-\tfrac{128}{81}q^4\cos^4\theta'] \times\left[1-\frac{1}{2\pi}\left(\frac{1}{\cos\theta'}\right)^{2in}\int_0^{2\pi}d\phi_s(1-\sin2\theta'\cos\phi_s)^{in}\right]\right\}. \tag{18}$$

Equation (18) shows that $F_{fi}(\vec{q})$ is independent of the scattering azimuth angle ϕ, as it should be in the present case of $1s-2s$ excitation. We have evaluated $F_{fi}(\vec{q})$ numerically from Eq. (18) by two independent methods which have yielded essentially identical results. Our first method involved computing the integral over ϕ_s numerically, and afterwards performing the second numerical integration over θ' (but, for convenience, first replacing θ' by the new integration variable t via $t=\sin\theta'$). In our second method we evaluated the integral over ϕ_s in (18) from the previously used[3] formula

$$(1/2\pi)\int_0^{2\pi}d\phi_s(1-\sin2\theta'\cos\phi_s)^{in} = |\cos2\theta'|^{2in+1}\;{}_2F_1(\tfrac{1}{2}in+\tfrac{1}{2},\tfrac{1}{2}in+1;1;\sin^22\theta'). \tag{19}$$

Equation (19) can be derived, e.g., by writing [when, as in (18), $0<\theta'<\frac{1}{2}\pi$]

$$1-\sin2\theta'\cos\phi_s = |\cos2\theta'|(|\sec2\theta'|-|\tan2\theta'|\cos\phi_s)$$

and then using a known integral representation[11] for the Legendre function, which is expressible[12] in terms of the hypergeometric function ${}_2F_1$.

To convert to cgs units, we replace K_i and q in (18) by a_0K_i' and a_0q', where the primed quantities are in cgs units (i.e., $K_i'=mv_i/\hbar$ in cgs units), and multiply the right-hand side of (18) by an extra factor a_0, consistent with F_{fi} having the dimensions of length.

B. 1s-3s Excitation

In atomic units, after we have introduced the 1s and 3s wave functions, Eq. (1) becomes

$$F_{fi}(\vec{q})=\frac{iK_i}{2\pi}\int\frac{1}{81\pi\sqrt{3}}\left(27+18\frac{\partial}{\partial\lambda}+2\frac{\partial^2}{\partial\lambda^2}\right)\times e^{-\lambda r}\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2in}\right]e^{i\vec{q}\cdot\vec{b}}(bdb\,d\phi_b)(sds\,d\phi_s\,dz) \tag{20}$$

evaluated at $\lambda=\frac{4}{3}$. Using Eqs. (11) and (17), we reduce Eq. (20) to

$$F_{fi}(\vec{q})=\frac{81}{64}\frac{iK_i}{\sqrt{3}}\int_0^{\pi/2}d\theta'\frac{\sin^3\theta'\cos\theta'}{(\sin^2\theta'+\frac{9}{16}q^2\cos^2\theta')^6}\times\{[-\sin^6\theta'-\tfrac{9}{8}q^2\sin^4\theta'\cos^2\theta' + (3^7/2^8)q^4\sin^2\theta'\cos^4\theta'-(3^7/2^{10})q^6\cos^6\theta'] \times[1-(2\pi)^{-1}(1/\cos\theta')^{2in} \times\int_0^{2\pi}d\phi_s(1-\sin2\theta'\cos\phi_s)^{in}]\}\,. \tag{21}$$

C. 1s-2p Excitation

The observed $1s$-$2p$ excitation cross section is the sum of the cross sections for excitation to each of the $2p$ magnetic substates. For our present purposes, the electron spin, $2p_{1/2}$-$2p_{3/2}$ splitting, and hyperfine effects all are inconsequential, so that the electrons can be considered spinless in effect, and the $2p$ magnetic substates can be labeled merely by the orbital magnetic quantum numbers $m=0,\pm1$. Let the direction of $\vec{K}_i$ (the z axis employed in Sec. II) be the axis of quantization for the atomic wave functions. Then for excitation to $m=0$, Eq. (1) yields

$$F_{fi}(\vec{q})=\frac{iK_i}{2\pi}\int\frac{1}{4\pi\sqrt{2}}re^{-\lambda r}\cos\theta_s\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2in}\right]\times e^{i\vec{q}\cdot\vec{b}}(bdb\,d\phi_b)(sds\,d\phi_s\,dz)\,, \tag{22}$$

where $z=r\cos\theta_s$ and $\lambda=\frac{3}{2}$. Thus $F_{fi}(\vec{q})$ from (22) vanishes, since it is integrated from $z=-\infty$ to $+\infty$ and the integrand is an odd function of z. It can be seen that this result – namely that $F_{fi}(\vec{q})$ vanishes for excitation to the $2p$ $m=0$ state – is a consequence of the Glauber-theory assumption that $\vec{q}$ is perpendicular to $\vec{K}_i$. In FBA, where one does not assume $\vec{q}\perp\vec{K}_i$, the $1s$-$2p$ $m=0$ excitation amplitude is not identically zero. However, examination of the quite complicated closed-form FBA expressions[13] for the $1s$-$2p$ $m=0,\pm1$ amplitudes indicates that (for those scattering angles making the predominant contribution to the excitation cross sections) the $m=0$ amplitude becomes negligible compared to the $m=\pm1$ amplitudes in the limit $E_i\to\infty$. This conclusion concerning the high-energy behavior of the FBA $1s$-$2p$ $m=0,\pm1$ amplitudes is supported by numerical calculations[14] which show that the FBA $1s$-$2p$ $m=0$ integrated cross section decreases much more rapidly than the FBA $1s$-$2p$ $m=\pm1$ integrated cross sections as the energy increases from 13 to 200 eV. Thus, the Glauber result that the $1s$-$2p$ $m=0$ amplitude vanishes is not inconsistent with the expectation (explained in Sec. II) that the Glauber total cross-section predictions should merge with the FBA at large E_i. We stress that the preceding sentence pertains to quantization along $\vec{K}_i$ only. In FBA it is more usual and more convenient to quantize along $\vec{q}$, in which event the FBA $1s$-$2p$ $m=\pm1$ amplitudes vanish, and the dominant FBA amplitude is the $1s$-$2p$ $m=0$.

For $1s$-$2p$ excitation to $m=1$,

$$F_{fi}(\vec{q})=\frac{iK_i}{2\pi}\int\frac{1}{8\pi}re^{-\lambda r}\sin\theta_s e^{i\phi_s}\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2in}\right]e^{i\vec{q}\cdot\vec{b}}(bdb\,d\phi_b)(sds\,d\phi_s\,dz) \tag{23}$$

with λ again $=\frac{3}{2}$; but since $r\sin\theta_s=s$, (23) can be rewritten

$$F_{fi}(\vec{q})=(iK_i/16\pi^2)\int ds\,db\,dz\,bs^2e^{-\lambda(s^2+z^2)^{1/2}}e^{i\phi_q}\int d\phi_b e^{i(\phi_b-\phi_q)}e^{i\vec{q}\cdot\vec{b}}\int d\phi_s e^{i(\phi_s-\phi_b)}[1-(|\vec{b}-\vec{s}|/b)^{2in}]\,. \tag{24}$$

Recalling (9), in (24), we obtain

$$\int_0^{2\pi}d\phi_s e^{i(\phi_s-\phi_b)}\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2in}\right]=-\left(\frac{2s}{bY}\right)^{in}\int_0^{2\pi}d\phi_s\cos\phi_s(1-Y\cos\phi_s)^{in}\,, \tag{25}$$

where Y is as in Eq. (12). Thus,

$$F_{fi}(\vec{q})=(K_ie^{i\phi_q}/8\pi)\int ds\,db\,dz\,bs^2e^{-\lambda(s^2+z^2)^{1/2}}J_1(qb)(2s/bY)^{in}\int_0^{2\pi}\cos\phi_s(1-Y\cos\phi_s)^{in}d\phi_s\,, \tag{26}$$

$$F_{fi}(\vec{q})=(K_ie^{i\phi_q}/4\pi)\int dsdb\,bs^3K_1(\lambda s)J_1(qb)(2s/bY)^{in}\int_0^{2\pi}d\phi_s\cos\phi_s(1-Y\cos\phi_s)^{in}\,. \tag{27}$$

As in Sec. III A, introducing polar coordinates in the b, s plane, reduces Eq. (27) to

$$F_{fi}(\vec{q}) = \frac{2^{12}K_i}{3^6\pi}\, q\, e^{i\phi_q}\int_0^{\pi/2} \frac{d\theta' \cos^2\theta' \sin^4\theta' (\sin^2\theta' - \frac{4}{9}q^2\cos^2\theta')}{(\sin^2\theta' + \frac{4}{9}q^2\cos^2\theta')^5}\left(\frac{1}{\cos\theta'}\right)^{2in}\int_0^{\pi} d\phi_s \cos\phi_s (1 - Y\cos\phi_s)^{in}\,, \tag{28}$$

where $Y = \sin 2\theta'$. We have computed $F_{fi}(\vec{q})$ numerically from (28), after having introduced the new integration variable $t = \sin\theta'$. Note that $F_{fi}(\vec{q})$ now depends on the scattering azimuth angle $\phi = \phi_q - \pi$, as foreshadowed in Sec. II. However, $|F_{fi}(\vec{q})|^2$ remains independent of ϕ. The quantity $|F_{fi}(\vec{q})|^2$ for $1s$-$2p$ $m = -1$ obviously is the same as for $m = 1$.

In (28), the integral over ϕ_s also can be expressed as a hypergeometric function. Using (19) and the properties[15] of the derivative of ${}_2F_1$, we obtain

$$\begin{aligned}\int_0^{\pi} d\phi_s \cos\phi_s (1 - Y\cos\phi_s)^{in} &= -\tfrac{1}{2}(in+1)^{-1}\frac{\partial}{\partial Y}\int_0^{2\pi} d\phi_s (1 - Y\cos\phi_s)^{in+1} \\ &= -\frac{\pi}{in+1}\frac{\partial}{\partial Y}\left[(1-Y^2)^{in+3/2}\, {}_2F_1(\tfrac{1}{2}in+1, \tfrac{1}{2}in+\tfrac{3}{2}; 1; Y^2)\right] \\ &= -\tfrac{1}{2}in\pi Y(1-Y^2)^{in+1/2}\, {}_2F_1(\tfrac{1}{2}in+1, \tfrac{1}{2}in+\tfrac{3}{2}; 2; Y^2)\,.\end{aligned}$$

D. $1s$-$3p$ Excitation

As in Sec. III C, the $1s$-$3p$ $m=0$ amplitude vanishes; also, the values of $|F_{fi}(\vec{q})|^2$ for $m = \pm 1$ are equal and independent of ϕ. For $1s$-$3p$ $m=1$, we find

$$\begin{aligned}F_{fi}(\vec{q}) = \frac{2^8 K_i q e^{i\phi_q}}{27\pi}\int_0^{\pi/2} \frac{d\theta' \cos^2\theta' \sin^4\theta'}{(\lambda^2\sin^2\theta' + q^2\cos^2\theta')^6}\, \{[\lambda^4(6\lambda-7)\sin^4\theta' + 12\lambda^2 q^2 \sin^2\theta' \cos^2\theta' - (6\lambda+1)q^4\cos^4\theta'] \\ \times [1/(\cos^2\theta')^{in}]\int_0^{\pi} d\phi_s \cos\phi_s (1 - \sin 2\theta' \cos\phi_s)^{in}\}\end{aligned} \tag{29}$$

evaluated at $\lambda = \frac{4}{3}$.

IV. RESULTS AND DISCUSSION

In Sec. IV A we concentrate on the total cross section for $1s$-$2s$ excitation. Subsequent subsections discuss $\sigma_{2p,1s}$, present the computed $\sigma_{3s,1s}$ and $\sigma_{3p,1s}$, and examine the predicted differential cross sections. Conclusions concerning the validity and utility of Glauber theory for computing excitation cross sections in electron-atom collisions, as evidenced by the results of this paper, are summarized in Sec. IV E.

A. Total $1s$-$2s$ Cross Section

Figure 2 compares our Glauber total $1s$-$2s$ excitation cross sections with a variety of previous theoretical estimates of $\sigma_{2s,1s}$. Specifically, Fig. 2 plots $\sigma_{2s,1s}$ versus E_i as computed via FBA[16] (curve 1); the second Born approximation,[17] in which, however, contributions from coupling to highly excited (principal quantum number $n > 5$) intermediate states have been estimated only approximately, using closure (curve 6); the distorted-wave approximation[18] (curve 7); a $1s$-$2s$-$2p$ close-coupling calculation, including exchange[19] (curve 5); FBA combined with the Ochkur approximation[20] for the exchange amplitude (curve 2); the so-called Vainshtein approximation[7] (curve 3); and finally the Glauber approximation (curve 4). It is seen that all methods give essentially the same results above 200 eV and that significant differences between the various approximations do not set in until the incident energy is decreased below 100 eV. We note that the Glauber predictions tend to lie below the others, especially at energies < 30 eV. In particular, the Glauber $\sigma_{2s,1s}$ is well below the FBA at energies < 100 eV; this behavior of the Glauber excitation cross section $\sigma_{2s,1s}$ contrasts with the behavior of the Glauber elastic $\sigma_{1s,1s}$, which exceeds the FBA $\sigma_{1s,1s}$ at all energies.[3]

Figure 3 compares the experimentally observed $1s$-$2s$ excitation cross sections with the Glauber predictions (solid curve). The solid circle data points are from the very recent measurements of Kauppila, Ott, and Fite (KOF).[21] The agreement between these observations and the Glauber theoretical values is quite good in the energy range above 30 eV. Referring to Fig. 2, it can be seen that except for the Vainshtein approximation the Glauber approximation is the only theoretical estimate which will be reasonably close to the data

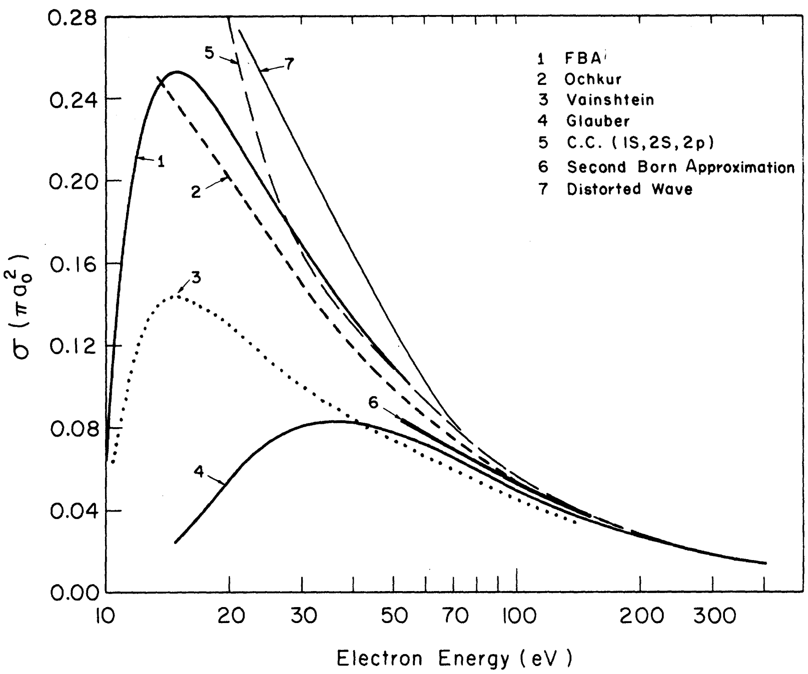

FIG. 2. The $1s$-$2s$ excitation cross section, in units of πa_0^2, computed via the Glauber and various other approximations discussed in the text. Curve 5 is the Burke, Schey, and Smith (Ref. 19) $1s$-$2s$-$2p$ close-coupling calculation, including exchange; curve 6 is the Holt and Moiseiwitsch (Ref. 17) estimate, using closure, of the second Born approximation; curve 7 is the distorted-wave approximation.

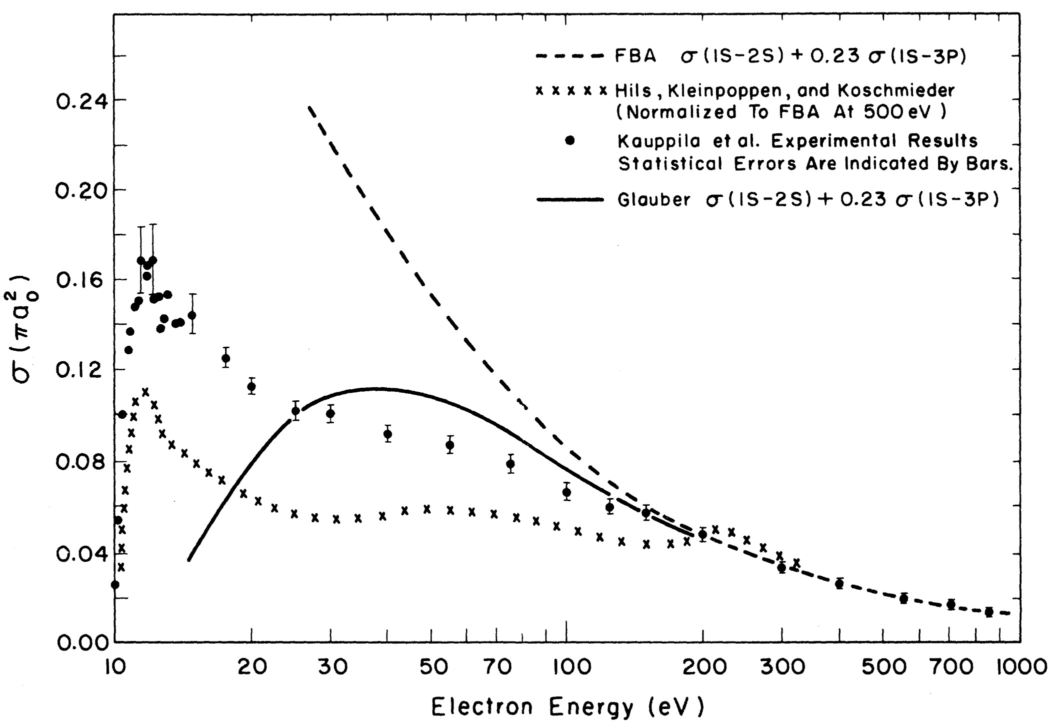

FIG. 3. Comparison of theoretical and experimental effective $1s$-$2s$ excitation cross sections in units of πa_0^2. Solid circles are data points of Ref. 21, normalized to FBA at 200 eV; crosses, the data points of Ref. 24, normalized to FBA at 500 eV. Solid curve, the Glauber predictions; dashed curve, the first Born approximation. As explained in the text, in order that comparison with the data be meaningful, the theoretical curves must plot $\sigma_{2s,1s} + \gamma\sigma_{3p,1s}$, where γ has been estimated to equal 0.23.

of Kauppila *et al.* in the energy range 30–100 eV; all other theories predict $\sigma_{2s,1s}$ cross sections which are much too high, e.g., the FBA (dashed curve in Fig. 3). Moreover, it is fair to say that the Vainshtein approximation rests on a very uncertain theoretical foundation, [22] in that calculations via this method incorporate subsidiary physically unjustified mathematical simplifications (e.g., a so-called peaking approximation) introduced solely for the purpose of making integrals tractable.

We also remark that although the magnitudes of the experimental cross sections have been in dispute for some years, [21,23] it seems unlikely that future experiments will yield observed $\sigma_{2s,1s}$ much larger than observed by Kauppila *et al.*, [21] i.e., it seems unlikely that future experiments will cause the Glauber approximation to look poorer than, e.g., the $1s$-$2s$-$2p$ close coupling (curve 5 of Fig. 2) in 30 eV $< E_i <$ 100 eV. The very careful experiments of KOF assume that $\sigma_{2p,1s}$ is correctly given by FBA at 200 eV, which is a perfectly reasonable assumption, judging by Fig. 4 below. Actually their results show that Kauppila *et al.* equally well could have normalized their inferred $\sigma_{2s,1s}$ to the Born approximation $\sigma_{2s,1s}$ at 200 eV, which energy should be high enough for the FBA $\sigma_{2s,1s}$ to be reliable, judging now by Fig. 2. Moreover, the KOF results lie above those reported by Hils, Kleinpoppen, and Koschmieder, [24] who normalized to FBA at the even higher energy of 500 eV. At very low energies, $E_i <$ 40 eV, there are $\sigma_{2s,1s}$ data by Lichten and Schulz, [25] which originally were reported to lie considerably higher than the KOF points of Fig. 3, but which were based on normalization to FBA at 40 eV, which clearly is too low an energy to rely on FBA. When the Lichten and Schulz data at 25 eV are renormalized so that they coincide with KOF at 25 eV (which in effect renormalizes the Lichten and Schulz data to FBA at 200 eV), the Lichten-Schulz and KOF cross sections are in quite good agreement[21] over the entire energy range $E_i <$ 40 eV, where the two experiments overlap.

Another remark worth making is that in the very low energy range 10.2 eV $< E_i <$ 13 eV, six-state $1s$-$2s$-$2p$-$3s$-$3p$-$3d$ close-coupling calculations (including exchange) have been carried out, [26] whose results are quite close[21] to the Lichten and Schulz data renormalized as described in the preceding paragraph. Furthermore, this inclusion of coupling to $n = 3$ states significantly decreases[26] the predicted $\sigma_{2s,1s}$ from their three-state $1s$-$2s$-$2p$ close-coupling values (curve 5 of Fig. 2). It is possible, therefore, that a six-state close-coupling calculation would satisfactorily agree with the KOF data points of Fig. 3, perhaps even over the entire range 10.2 eV $< E_i <$ 200 eV. At the present time this possibility cannot be verified however; because the computations are so tedious, no six-state close-coupling calculations of $\sigma_{2s,1s}$ at energies $E_i >$ 13 eV have been carried out. Thus, for close-coupling predictions at $E_i >$ 13 eV, one is forced to fall back on the obviously inadequate (for energies 13 eV $< E_i <$ 100 eV) three-state $1s$-$2s$-$2p$ results. [19] Actually, the success of the Glauber approximation in Fig. 2, if not fortuitous, suggests that the close-coupling method is much more elaborate than necessary, for predicting $\sigma_{2s,1s}$ in the energy range $E_i >$ 30 eV at any rate; certainly the Glauber diffraction approximation ignores the interchannel coupling (supposedly capable of causing many successive excitations and deexcitations during the incident electron's transit of the target hydrogen atom) whose inclusion so greatly complicates the close-coupling computations.

As explained in Sec. II, the Glauber curve of Fig. 3 perforce neglects electron exchange. Therefore, the Glauber theory's apparent success for $\sigma_{2s,1s}$ excitation indeed would be fortuitous if neglect of exchange were unjustified above 30 eV. Various theoretical calculations[27] indicate that exchange should be quite negligible at incident energies $E_i >$ 100 eV, but may become fairly important at $E_i <$ 50 eV. Unfortunately, there are no very reliable means of quantitatively determining exchange contributions to cross sections at those low energies where exchange is likely to be nonnegligible. However, we have employed the Born-Oppenheimer (BO) approximation[27] to estimate the exchange amplitude in $1s$-$2s$ excitation. In this $1s$-$2s$ case, including the BO exchange amplitude along with the Glauber direct amplitude alters the solely Glauber predictions by only a few percent for 40 eV $< E_i <$ 70 eV and all consequential scattering angles (angles making nonnegligible contributions to the integrated cross section); above 100 eV the exchange contribution estimated in BO is utterly negligible, as far as the integrated cross section is concerned. Similar comments pertain to use of the Ochkur approximation for the exchange amplitude. [20] Below 40 eV, the BO exchange amplitude becomes more important compared to the Glauber direct amplitude, but in this energy range the BO amplitude tends to overestimate the exchange contribution, as is well known. [27] We conclude that neglect of exchange in the Glauber curve of Fig. 3 is justified in the energy range $E_i >$ 30 eV, where the Glauber approximation fits the KOF data. Neglect of exchange may be a reason, though not the sole possible reason (see Sec. IV E), for the apparent failure of the Glauber theory at $E_i <$ 30 eV in Fig. 3.

The measurements plotted in Fig. 3 do not distinguish between H(2s) atoms created by 1s-2s excitation and those produced by radiative cascading to H(2s) after excitation to higher levels, e.g., H(4p). Therefore the effective $\sigma_{2s,1s}$ observed in the experiments quoted in Fig. 3 must be

$$\sigma^{\text{eff}}_{2s,1s} = \sigma_{2s,1s} + \sum_j P(j \to 2s)\,\sigma_{j,1s} \tag{30}$$

summed over all energetically accessible levels j lying above H(2s), with $P(j\to 2s)$ the probability of cascading to H(2s) after initial excitation to H(j). The predominant cascade mechanism to H(2s) is via excitation to H(3p), i.e., the largest term in the above sum corresponds to $j = 3p$. Thus it is customary to rewrite (30) in the more convenient form

$$\sigma^{\text{eff}}_{2s,1s} = \sigma_{2s,1s} + \gamma\sigma_{3p,1s}\,, \tag{31}$$

where γ is computable from known transition probabilities[28] combined with estimates of the ratios $\sigma_{j,1s}/\sigma_{3p,1s}$. It seems to be generally agreed,[21,24] on the basis of Hummer and Seaton's[29] FBA estimates of these ratios, that $\gamma = 0.23$ over a broad range of energies. Consequently the theoretical curves in Fig. 3 are plots of the right-hand side of (31), using $\gamma = 0.23$. To be quite specific, in the dashed curve of Fig. 3 we use the FBA values of $\sigma_{2s,1s}$ and $\sigma_{3p,1s}$; in the solid Glauber curve we use $\sigma_{2s,1s}$ from Fig. 2 and the Glauber $\sigma_{3p,1s}$ from Fig. 6 below.

Actually, we have recomputed γ, using a somewhat more extensive set[16] of computed FBA cross sections than was available to Hummer and Seaton.[29] We find γ indeed is very nearly constant over the energy range of interest in Fig. 3, but that $\gamma = 0.19$ rather than 0.23. Use of this smaller value of γ makes the agreement between the Glauber theory and the KOF data even better than is shown in Fig. 3; however, because we have no prior assurance that the Glauber-predicted $\sigma_{2s,1s}$ and $\sigma_{3p,1s}$ are very accurate at $E_i > 30$ eV, we do not wish to conclude that $\gamma = 0.19$ is nearer the truth than $\gamma = 0.23$ when the exact $\sigma_{2s,1s}$ and $\sigma_{3p,1s}$ are used in Eq. (31). We add that if (as we claim) Glauber theory really is much superior to FBA, then the ratios $\sigma_{j,1s}/\sigma_{3p,1s}$ used to compute γ should be estimated from Glauber calculations, not from FBA. After $j = 3p$, the most important contributors (in FBA) to the sum in (30) are the $j = np$ terms, $n > 3$. We have not computed the Glauber $\sigma_{np,1s}$ for $n > 3$, so that we cannot immediately test the validity of the FBA-estimated $\sigma_{np,1s}/\sigma_{3p,1s}$ for $n > 3$. However, our computations do enable us to compare the FBA and Glauber ratios $\sigma_{np,1s}/\sigma_{2p,1s}$. We find that these ratios are very nearly equal at energies $E_i > 30$ eV. Therefore, for energies exceeding 30 eV at any rate, estimates of γ in (31) from the FBA ratios $\sigma_{j/1s}/\sigma_{3p,1s}$ should be quite accurate.

B. Total 1s-2p Cross Sections

In Fig. 4 we compare theoretical and experimental values of the total 1s-2p excitation cross section. The sources and descriptions of the theoret-

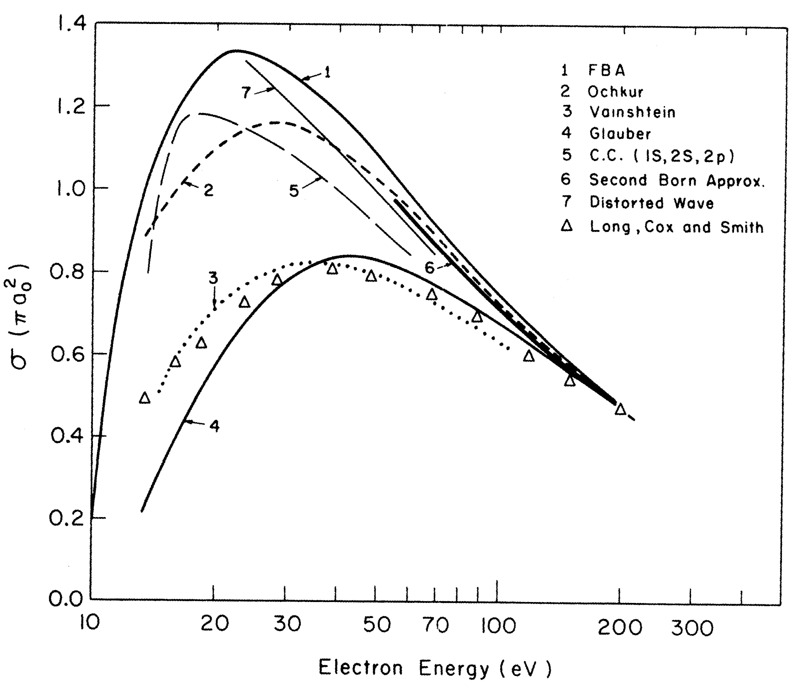

FIG. 4. 1s-2p excitation cross section in units of πa_0^2. The triangles are the data points of Ref. 30. The curves show various theoretical estimates of 1s-2p excitation, computed via the Glauber and various other approximations discussed in the text. The sources for the theoretical curves are as in Fig. 2, e.g., curve 5 is the 1s-2s-2p close-coupling calculation, including exchange, from Ref. 19.

ical curves in Fig. 4 are the same as those cited in connection with Fig. 2 above, e.g., curve 6 in Fig. 4 is the Holt and Moiseiwitsch[17] second Born approximation for $\sigma_{2p,1s}$, in which, however, contributions to highly excited ($n > 5$) intermediate states have been estimated only approximately, using closure. As in the $1s$-$2s$ case, all theories are fairly close for $E_i > 100$ eV; for $E_i < 100$ eV the Glauber approximation tends to be significantly lower than other theoretical calculations, excepting the Vainshtein approximation (curve 3). The triangles in Fig. 4 are the experimental data points of Long, Cox, and Smith (LCS),[30] which are the most recent measurements of $\sigma_{2p,1s}$ and which are in good agreement with older experiments.[31,32] Because cascading is estimated[30] to make only a 2% contribution to the observed $\sigma_{2p,1s}$, in Fig. 4 it is legitimate to compare the observed data points with theoretical curves uncorrected for cascading (as would not have been legitimate in Fig. 2). Again we see that the Glauber theory is in good agreement with experiment at energies $E_i > 30$ eV, but is rather lower than observed for $E_i < 30$ eV. In particular, at energies 30 eV $< E_i < 100$ eV, the Glauber approximation is distinctly superior to all other theoretical calculations shown in Fig. 4, excluding the not-well-founded Vainshtein approximation.

Actually, the data points shown in Fig. 4 have had to be computed from the values reported by LCS,[30] because those observers, as well as previous workers,[31,32] only measure $Q_\perp$, defined as 4π times the number of Lyman-α photons per unit solid angle emitted in a direction perpendicular to the direction of the incident electron beam, normalized at 200 eV to the number expected from FBA. The total cross section σ to be plotted in Fig. 4 is given in terms of $Q_\perp$ by[33]

$$\sigma = (1 - \tfrac{1}{3}P)Q_\perp \,, \tag{32}$$

where the polarization fraction P has its customary definition

$$P = (I_\parallel - I_\perp)/I_\parallel + I_\perp) \tag{33}$$

in terms of the intensities, observed at 90° to the electron beam axis, of the Lyman-α components having electron vectors parallel and perpendicular to the electron beam axis. Values of $P(E_i)$ have been measured recently by Ott, Kauppila, and Fite.[33] Using these values in (32), together with the normalized $Q_\perp(E_i)$ reported by LCS, yields the data points plotted in Fig. 4.

Recently there has been much interest in the Gryzinski[34] classical model for prediction of atomic collision cross sections. The Gryzinski predictions have the virtue of easy computability, even easier than the FBA and the Glauber approximation. However, the Gryzinski prescription[34] for computing excitation cross sections yields only the total cross section for excitation to the $n = 2$ levels of atomic hydrogen; the Gryzinski formulation does not distinguish between excitation to degenerate (or nearly degenerate) levels of different orbital angular momentum. For this reason, in Fig. 5 we have plotted theoretical and experimental values of the total cross section for excitation to the hydrogen $n = 2$ levels. The solid curve is the sum of the Glauber curves (curves 4) in Figs. 2 and 4; the dashed curve is the similar sum of the FBA curves (curves 1) in Figs. 2 and 4; the dot-dashed curve is the Gryzinski prediction, as computed by Stabler.[35] The triangles in Fig. 5 are the data, obtained by adding the solid circles in Fig. 3 to the triangles in Fig. 4. Evidently the Glauber approximation yields a much better fit than the Gryzinski model; however, the trivial Gryzinski computation does correctly predict the peak-combined cross section $(\sigma_{2s,1s} + \sigma_{2p,1s})$ to within 50%. We note that in adding the experimental points of Figs. 3 and 4 we are including the contribution from cascading to H($2s$), which contribution is not included in the theoretical curves of Fig. 5. On the other hand, the experimental points in Fig. 3 lie much lower than those in Fig. 4, i.e., the experimental (and theoretical) curves in Fig. 5 are dominated by $\sigma_{2p,1s}$; consequently, subtraction of the cascading contribution from the

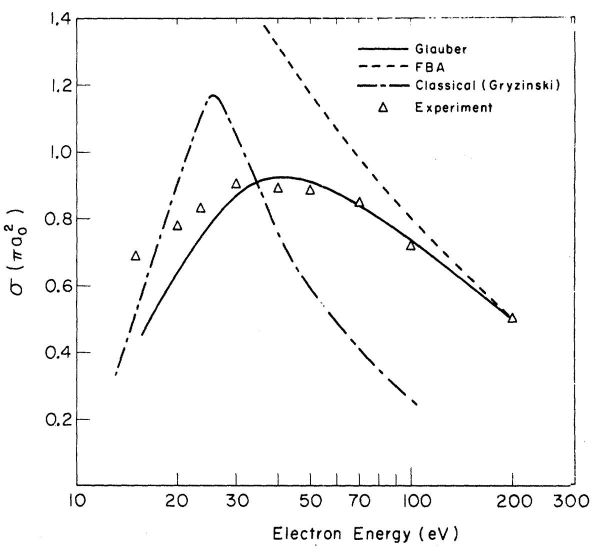

FIG. 5. Total cross section for excitation to the $n = 2$ levels of hydrogen, in units of πa_0^2. The triangles are the observations, taken from Figs. 3 and 4 as explained in the text. Solid curve, the Glauber predictions, from Figs. 3 and 4; dashed curve, the first Born approximation, from Figs. 3 and 4; dot-dashed curve, the Gryzinski classical model, as computed in Ref. 35.

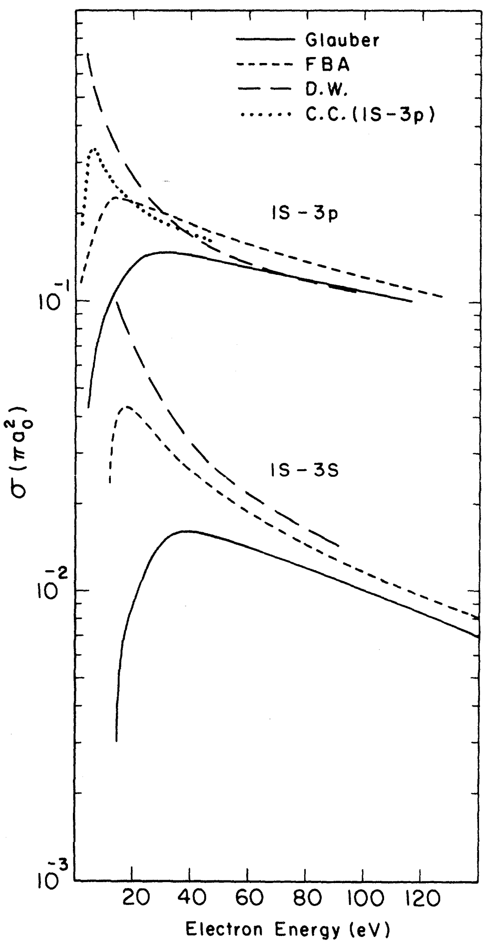

FIG. 6. Theoretical $1s$-$3s$ and $1s$-$3p$ cross sections in units of πa_0^2. Solid curves are the Glauber predictions; short dashed curves, the first Born approximation; long dashed curves, the distorted-wave approximation; dotted curve, a $1s$-$3p$ close-coupling calculation (Ref. 19).

experimentally observed H($2s$) production would only slightly modify the experimental points of Fig. 5.

C. Total $1s$-$3s$ and $1s$-$3p$ Cross Sections

In Fig. 6 are displayed the Glauber predictions for $\sigma_{3s,1s}$ and $\sigma_{3p,1s}$ (solid curves), together with FBA[16] (short dashes) and distorted-wave[18] (long dashes) calculations; in addition, for $1s$-$3p$ excitation alone, there are shown results computed in a two-state $1s$-$3p$ close-coupling approximation,[19] including exchange. There are no reliable data with which these predictions can be compared. The relations between the various curves in Fig. 6 are much the same as were found for the corresponding curves of Figs. 2 and 4.

D. Differential Cross Sections

As yet we have not discussed differential cross-section predictions; these are shown in Fig. 7, for excitation to $2s$, $2p$, $3s$, and $3p$ at an incident electron energy of 100 eV. In Fig. 7, the solid curves are the Glauber results; the dashed curves are FBA differential cross sections, taken from Mott and Massey.[36] The absolute differential cross sections are plotted in Fig. 7, with the scale on the left referring to the $1s$-$2s$ and $1s$-$3s$ curves, while the scale on the right pertains to the $1s$-$2p$ and $1s$-$3p$ curves. The scales in Fig. 7 are much more condensed than those employed in Figs. 2, 4, and 6, so that, e.g., the differences between the FBA and Glauber $1s$-$2p$ curves in Fig. 7 do account for the roughly 10% difference between the FBA and Glauber total $\sigma_{2p,1s}$ curves of Fig. 4 at 100 eV.

As in e-H elastic scattering,[3,4] the Glauber and FBA curves of Fig. 7 all decrease monotonically with increasing scattering angle θ. In a number of other respects, however, the relations between corresponding Glauber and FBA curves of Fig. 7

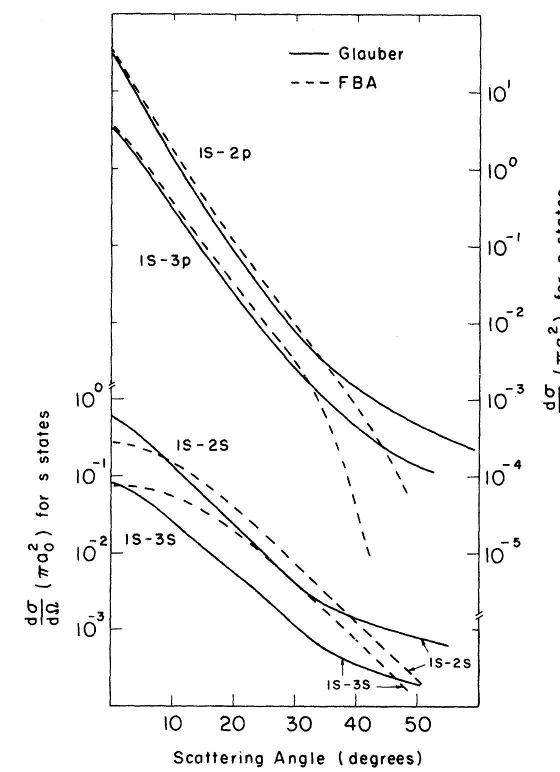

FIG. 7. Theoretical differential cross sections in units of πa_0^2 for excitation to $2s$, $2p$, $3s$, and $3p$, at 100 eV. Solid curves are the Glauber predictions; dashed curves, the first Born approximation.

are rather different from those for elastic scattering. At large angles, $\theta >\sim 40°$, the Glauber inelastic differential cross sections are significantly larger than the FBA; in elastic scattering at large angles the FBA and the Glauber approximation were practically indistinguishable,[3,4] but if anything, the FBA exceeded the Glauber. In elastic scattering at angles $0° < \theta <\sim 40°$, the Glauber approximation always exceeded the FBA, with the difference between the FBA and the Glauber approximations becoming quite large at very small angles $\theta <\sim 10°$; as a result, the Glauber total elastic cross section $\sigma_{1s,1s}$ exceeded[3] the FBA $\sigma_{1s,1s}$. On the other hand, in the 100-eV differential cross sections of Fig. 7, the Glauber $1s$-$2s$ curve only slightly exceeds the FBA $1s$-$2s$ in the angular range $\theta < 10°$, while at intermediate angles $10° < \theta < 40°$ the Glauber $1s$-$2s$ lies significantly below the FBA; consequently, recalling that in computing the total cross section the differential cross section $d\sigma/d\Omega$ is weighted by an extra factor $\sin\theta$, it is understandable that the Glauber total inelastic $\sigma_{2s,1s}$ turns out to be less than the FBA $\sigma_{2s,1s}$ at 100 eV, as was shown in

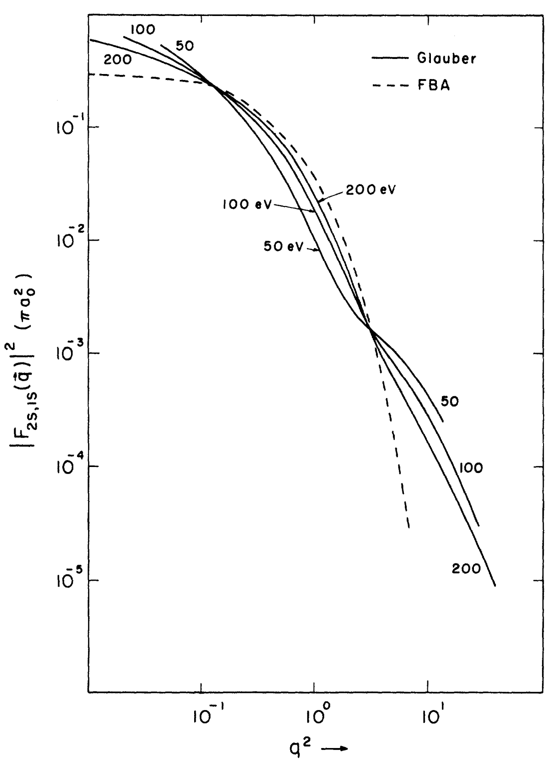

FIG. 8. Scattering amplitude squared in units of πa_0^2 for $1s$-$2s$ excitation, as a function of q^2 = momentum transfer squared. Solid curves are the Glauber predictions at energies of 50, 100, and 200 eV; dashed curve, the first Born approximation, which is independent of incident energy.

Fig. 2. In the $1s$-$3s$ case, the Glauber $d\sigma/d\Omega$ of Fig. 7 starts out only very slightly above the FBA at 0° and falls below the FBA at an angle θ as small as 2°. The $1s$-$2p$ and $1s$-$3p$ Glauber curves of Fig. 7 lie below their corresponding FBA curves even at 0°.

The features of the foregoing comparisons between the Glauber approximation and FBA inelastic differential cross sections are quite characteristic, i.e., these features appear to persist at essentially all energies $10 \text{ eV} < E_i < 200 \text{ eV}$. In general the differences between the Glauber approximation and the FBA inelastic $d\sigma/d\Omega$ become more marked at consequential angles (angles contributing significantly to the integrated cross section) as the energy is decreased. To illustrate this remark, in Fig. 8 we plot $|F_{2s,1s}(\vec{q})|^2$ from Eq. (18) as a function of q^2 for incident energies of 50, 100, and 200 eV (solid curves); for comparison the FBA $|F_{2s,1s}(\vec{q})|^2$, which is independent of incident energy, also is shown (dashed curve). For given E_i, $q^2(\theta)$ is a monotonically increasing function of scattering angle θ, but the value of q^2 at 0° increases as the incident energy decreases, e.g., at $E_i = 100$ eV, $q^2(0°) = 0.02$, while at $E_i = 50$ eV, $q^2(0°) = 0.04$. Moreover, in the range $10^{-1} < q^2 <\sim 3$ the Glauber curves lie below the Born, the more so as E_i decreases. Thus the fact that in Fig. 2 the FBA $\sigma_{2s,1s}$ lies increasingly above the Glauber $\sigma_{2s,1s}$ as the energy is decreased from 200 to about 20 eV also can be understood from Fig. 8, recalling that in computing the total cross section via Eq. (7) the quantity $|F_{fi}(\vec{q})|^2$ in the integrand is weighted by an extra factor q, while the lower integration limit is $[q^2(0°)]^{1/2}$. Below about 20 eV the Glauber approximation and the FBA $\sigma_{2s,1s}$ again approach each other in Fig. 2 because the integration range K_i-K_f to K_i+K_f in Eq. (7) rapidly diminishes as threshold $K_f = 0$ is approached.

The only angular distribution data with which our Glauber predictions can be compared are those of Williams,[37] who has measured the angular distribution of those scattered electrons whose energy loss corresponds to excitation of the $n = 2$ levels of atomic hydrogen. Figure 9 shows Williams's data points (labeled 1) at an incident electron energy $E_i = 50$ eV, normalized at 20° to the sum of the cross sections for excitation of H($2s$) and H($2p$), as calculated (at 54 eV) by Scott[38] in the $1s$-$2s$-$2p$ close-coupling approximation. Curves 2 and 3 in Fig. 9 also are taken directly from Williams.[37] Curve 2 shows the aforementioned $1s$-$2s$-$2p$ close-coupling predictions[38]; curve 3 shows the (BO) predictions (again at 54 eV), also normalized at 20° to the observations. As Williams remarks, at angles $\theta <\sim 80°$ the BO curve

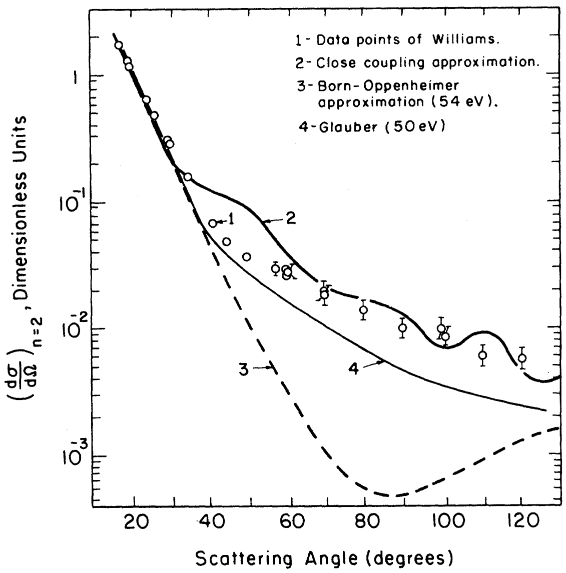

FIG. 9. Differential cross sections for excitation of the $n=2$ levels of atomic hydrogen. Curve 1 fits data points of Williams, Ref. 37. Curves 2–4 are theoretical angular distributions, all normalized to the experimental data points at $\theta=20°$. Curve 2, the $1s$-$2s$-$2p$ close-coupling predictions; curve 3, the Born-Oppenheimer approximation; curve 4, the Glauber approximation.

is essentially identical with the FBA. At angles $\theta > 80°$ the effects of electron exchange cause the BO curve to turn up; the FBA, which neglects exchange, continues to decrease monotonically as θ increases beyond 80°, consistent with our discussion of Fig. 7. Curve 4 of Fig. 9 displays the Glauber predictions for $E_i = 50$ eV normalized (like the other theoretical curves) to the data points at 20°. At angles $20° < \theta < 40°$ there is not much to choose between the various theories. For $\theta > 40°$ the $1s$-$2s$-$2p$ close-coupling gives a quite good fit, while the FBA or BO are clearly bad fits. The Glauber approximation is not quite as good as the $1s$-$2s$-$2p$ close coupling at $\theta > 40°$, but the Glauber fit certainly is not poor. It will be recalled that the $1s$-$2s$-$2p$ close-coupling calculations, although much more arduous than the Glauber approximation, at 50 eV actually predicted much less accurate total $\sigma_{2s,1s}$ and $\sigma_{2p,1s}$ than did the Glauber (Figs. 2–4).

Figure 10 compares Williams's data[37] (curves 1) with theoretical angular distributions at incident electron energies of 100 eV [Fig. 10(a)] and 200 eV [Fig. 10(b)]. At these energies since there are no close-coupling calculations, Williams fitted his observations to the BO (curves 2) at 21°. As was the case at 50 eV, these 100- and 200-eV BO curves are bad fits to the observed points. In addition, Fig. 10 shows the Glauber predictions (curves 3), also normalized to Williams's data points at 21°. At 100 eV the Glauber approximation yields an acceptable fit; at 200 eV the Glauber fit is excellent. It is noteworthy that at fixed large angle (e.g., $\theta = 60°$) the deviation between the Glauber approximation and the FBA increases with increasing energy in Figs. 9 and 10, contrary to the (now seen to be dubious) inference in

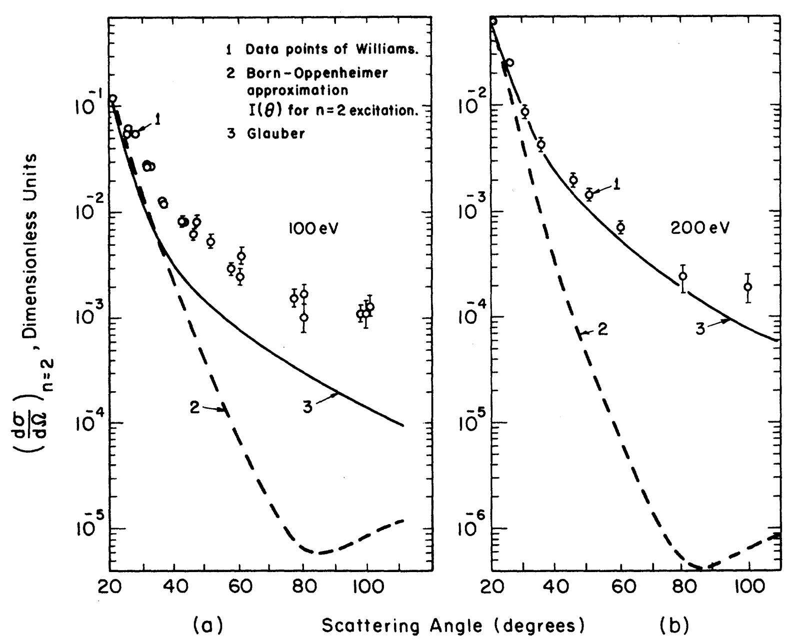

FIG. 10. Differential cross sections for excitation of the $n=2$ levels of atomic hydrogen (a) at 100 eV; (b) at 200 eV. Curves 1 fit data points of Ref. 37. Curves 2 and 3 are theoretical angular distributions, all normalized to the experimental data points at $\theta=21°$. Curve 2 (dashed), the Born-Oppenheimer approximation; curve 3 (solid), the Glauber approximation.

Sec. II that the Glauber $F_{fi}(\vec{q})$ should approach the Born $F_{fi}(\vec{q})$ at high energies. We add that excepting backward angles, where the BO amplitudes approach the Glauber amplitudes, inclusion of electron exchange could not significantly modify any of the Glauber curves in Figs. 9 and 10.

Of course, 200 eV is not really a high enough energy to justify retaining only the leading term in the expansion of the exponential in (2); in fact, at 200 eV the expansion parameter $2n$ in Eqs. (2) and (3) equals $\frac{1}{2}$. In other words, at 200 eV the energy is still too low for our confidence in the argument – via expansion of $e^{i\chi}$ in (2) – which seemingly reduces the formula [Eq. (1)] to the FBA scattering amplitude. Still, $2n$ is not large compared to unity at 200 eV; moreover, it is curious that the Glauber approximation and the FBA should be so divergent at wide angles in Fig. 10(b), in view of the fact that for elastic scattering the 200-eV Glauber approximation and FBA predictions are indistinguishable[4] for angles exceeding 30°. We stress that even without normalization to the same value at $\theta = 21°$, the FBA and Glauber integrated cross sections from Fig. 10(b) will be practically equal, as we already know from Figs. 2 and 4 at 200 eV. In other words, the angles where the FBA and Glauber curves of Fig. 10(b) diverge widely are quite inconsequential for computing the 200-eV total cross section for excitation to the H $n = 2$ levels, as can be directly verified from Fig. 10(b) (and its extrapolation to $\theta = 0°$).

For the purposes of Sec. IV E, it is desirable that we assure ourselves that the divergence at large scattering angles between the FBA and Glauber angular distributions of Fig. 10 is consistent with Fig. 8. At $E_i = 200$, or 100 eV, the FBA and Glauber $|F|^2$ shown in Fig. 8 lie close to each other only for $q^2 <\sim 3$; at larger q^2 the FBA $|F|^2$ becomes very small compared to the Glauber $|F|^2$. Now at 200 eV, $q^2(\theta)$, which increases monotonically with θ at fixed E_i, equals 3 at about $\theta = 25°$. Thus the angular range for which the FBA and the Glauber approximation predict very nearly the same $1s$-$2s$ differential cross sections at 200 eV is largely off-scale in Fig. 10(b). At 100 eV, $q^2(\theta) = 3$ at about $\theta = 40°$, so that curves 2 and 3 in Fig. 10(a) do not begin to diverge until θ exceeds 40°. Actually, it is not possible to understand Figs. 10(a) and (b) solely from the $1s$-$2s$ curves of Fig. 8, because $1s$-$2p$ excitation contributes importantly to Fig. 10. However, the variation with q^2 of the $1s$-$2p$ $d\sigma/d\Omega$ is not qualitatively dissimilar from the corresponding variation of the $1s$-$2s$ $d\sigma/d\Omega$, as Fig. 7 indicates, so that concentrating solely on the behavior of the $1s$-$2s$ curves of Fig. 8 does yield qualitatively correct interpretations of Figs. 10(a) and (b).

E. Conclusions and Critique

From the results which have been discussed it is legitimate to conclude that the Glauber theory is a useful, fairly accurate means of predicting total cross sections for excitation of atomic hydrogen by electrons at energies 30 eV $< E_i <$ 200 eV; in fact, in this energy range, if theories of e – H excitation are judged on any reasonably weighted combination of reliability, ready computability, and theoretical soundness, no other theory seems at all competitive with the Glauber theory. Whether similar conclusions would hold for other atoms and other incident projectiles, e.g., e-He and p-H collisions, is a question well worth investigating. For instance, in many electron atoms, where $F_{fi}(\vec{q})$ from Eq. (1) must be integrated over the coordinates $\vec{r}_1, \vec{r}_2, \ldots,$ of all the atomic electrons, it is far from obvious that $F_{fi}(\vec{q})$ can be reduced to a readily computable form without subsidiary error-introducing, simplifying mathematical approximations.

The angular distribution results we have quoted certainly justify the conclusion that the potential utility of Glauber theory for predictions of inelastic (as well as elastic) differential cross sections in electron-atom collisions cannot be lightly dismissed. As a matter of fact, judging by Figs. 9 and 10, Glauber predictions of differential cross sections, for e-H excitation in the same energy range 30 eV $< E_i <$ 200 eV, are almost as successful as are the Glauber total cross-section predictions. At first sight, this last assertion is rather surprising. In Figs. 9 and 10 the main advantage of the Glauber approximation lies in its ability to predict the observed angular distributions at wide scattering angles, where the BO and FBA differential cross sections are far too low; at smaller angles, as Figs. 7–10 indicate, normalized (not absolute) differential cross sections are fitted no better by the Glauber approximation than by the even more readily computable FBA. However, as explained in Sec. II, our calculations specifically have assumed that the momentum transfer $\vec{q}$ is perpendicular to $\vec{K}_i$; i.e., that $\vec{q}$ in Eqs. (1) or (8) lies in the x, y plane containing $\vec{b}$ and $\vec{s}$. Whether or not the incident energy is high, $\vec{q}$ cannot be perpendicular to $\vec{K}_i$ at the wide angles where FBA fails in Figs. 9 and 10. In other words, it appears that the Glauber predictions are successful in Figs. 9 and 10 at just those angles where Glauber theory might be expected to break down.

On the other hand, the foregoing objection to Glauber theory is specious. In Glauber theory, the phase distortion of the wave function is approximated via integration along a straight line supposedly representing the undeviated path of the incident electron; this is how one arrives at the formula for χ [Eqs. (2)–(3)]. For wide-angle scattering, as Glauber remarks[1,2], a poor approximation results from supposing that the electron path is always parallel to $\vec{K}_i$. A better approximation, which treats the initial and final directions symmetrically, results from the assumption that the electron's undeviated straight-line path effectively is parallel to $\frac{1}{2}(\vec{K}_i+\vec{K}_f)$. However, recalling Eqs. (6), we have

$$\frac{\vec{q}\cdot(\vec{K}_i+\vec{K}_f)}{|\vec{q}\,|\,|\vec{K}_i+\vec{K}_f|}=\frac{K_i^2-K_f^2}{q|\vec{K}_i+\vec{K}_f|}$$

$$=\frac{2m(\epsilon_f-\epsilon_i)/\hbar^2}{[(K_i^2+K_f^2)^2-4K_i^2K_f^2\cos^2\theta]^{1/2}}$$

$$=\frac{\epsilon_f-\epsilon_i}{[(\epsilon_f-\epsilon_i)^2+4E_iE_f\sin^2\theta]^{1/2}}\quad. \tag{34}$$

Thus, at large scattering angles (not too near $\theta=180°$), choosing the z axis along $\frac{1}{2}(\vec{K}_i+\vec{K}_f)$ automatically implies that $\vec{q}$ very nearly lies in the x, y plane at not exceedingly low energies. For example, in $1s$-$2p$ excitation at $E_i=200$ eV, the right-hand side of (34) $=\sim 0.05$ for $\theta=30°$. Moreover, at any given fixed scattering angle it can be seen that $\sum|F_{fi}(\vec{q},m_f)|^2$ summed over all final magnetic quantum numbers m_f does not depend on the direction of quantization of the final bound-state wave functions $u_f(m_f)$. Therefore, the Glauber differential and integrated $e-\mathrm{H}(1s)$ cross sections we have computed are exactly the same as we would have obtained if, at the very beginning, back in Eq. (1), we had made the (superior at all not exceedingly low energies) supposition that the z axis lies along $\frac{1}{2}(\vec{K}_i+\vec{K}_f)$.

The preceding paragraph has made it understandable that Glauber theory accurately predicts differential cross sections at wide angles and not exceedingly small incident energies. It also is possible to understand the fact remarked in Sec. IV D that at wide angles the Glauber and FBA elastic differential cross sections[3,4] approach each other with increasing E_i, whereas the Glauber and FBA inelastic $d\sigma/d\Omega$ apparently are increasingly divergent with increasing E_i. At high energies, large-angle elastic scattering of electrons from H($1s$) results predominantly from close collisions between the incident electron and the proton; the atomic electron has too small a mass (alternatively, has too spread out a wave function) to give large deflections to the incident electron. Similarly, one expects that wide-angle inelastic scattering results from interactions of the incident electron with the proton as well as with the atomic electron. In FBA, however, the inelastic scattering produced by the interaction e^2/r' between the incident electron and the proton vanishes because the initial and final bound-state wave functions are orthogonal. Therefore the wide-angle inelastic scattering in FBA results only from the relatively ineffective electron-electron interaction, which explains why the FBA angular distributions of Figs. 9 and 10 decrease so much more rapidly with increasing angle than do the corresponding[3,4] FBA elastic $d\sigma/d\Omega$. This artificial and misleading elimination of the e^2/r' interaction does not occur in the Glauber approximation. Consequently, one expects, and finds, as comparison of Figs. 9 and 10 with Fig. 1 of Tai *et al.*[4] shows, that at any given energy the Glauber wide-angle inelastic and elastic $d\sigma/d\Omega$ decrease at about the same rate with increasing angle; the fact that at a given energy the experimental elastic and inelastic $d\sigma/d\Omega$ resemble each other already has been remarked by Williams.[37] Returning to the expansion of $e^{i\chi}$ in powers of χ, it appears from the previously reported calculations[3,4] and from the foregoing discussion that at $E_i>200$ eV keeping only the linear term in χ is not too bad for wide-angle elastic scattering. But for inelastic scattering at a fixed large angle, where the contribution from the electron-electron interaction decreases so rapidly with increasing E_i, the linear term in χ is not really the leading term in the expansion of $e^{i\chi}$ after removal of the e^2/r' interaction by orthogonality, and the Glauber approximation does not approach the FBA as E_i increases. It is relevant to later discussion to note here that when retention of only the linear term in χ is justified, the Eq. (1) reduces to FBA for each final magnetic sublevel, whatever the quantization direction of the atomic bound states, and whether or not the assumption $\vec{q}\cdot\vec{K}_i=0$ is valid.

For the inelastic collisions of interest in this paper, where $K_f<K_i$, the assumption that $\vec{q}$ is very nearly perpendicular to $\vec{K}_i$ fails at small scattering angles as well as at large θ. To make these remarks more specific, we write

$$\vec{q}=\vec{q}_{\parallel}+\vec{q}_{\perp},$$

where $\vec{q}_{\parallel}$ lies along $\vec{K}_i$, and $\vec{q}_{\perp}$ is the component of $\vec{q}$ perpendicular to $\vec{K}_i$. In terms of θ

$$q_{\parallel}=K_i-K_f\cos\theta,\quad q_{\perp}=K_f\sin\theta\ .$$

In elastic scattering, where $K_f=K_i$, it is evident that $q_{\parallel}$ becomes negligible compared to $q_{\perp}$ as $\theta\to 0$, i.e., in elastic scattering the assumption $\vec{q}\cdot\vec{K}_i=0$ is increasingly valid as $\theta\to 0$ at fixed E_i. When $K_f<K_i$, however, $q_{\perp}/q_{\parallel}\to 0$ as $\theta\to 0$ at fixed E_i, i.e., the vector $\vec{q}$ now becomes increasingly

parallel to $\vec{K}_i$ in this limit. Furthermore, as Eq. (34) shows, at small angles and moderate to low energies, failure of the assumption $\vec{q}\cdot\vec{K}_i=0$ cannot be remedied by using $\frac{1}{2}(\vec{K}_i+\vec{K}_f)$ as the z direction. One can argue that at large K_i the angular range near $\theta=0$, where $q_\parallel \ll q_\perp$ fails, is too small to make a consequential contribution to the integrated inelastic cross section. As K_i decreases, however, $q_\parallel \ll q_\perp$ is invalid in an increasing angular range near $\theta=0$, and eventually this range becomes large enough to be consequential in the integrated cross section. It is probable that this failure of the fundamental assumption $\vec{q}\cdot\vec{K}_i=0$ near $\theta=0$ is associated with the rapid dropoff of the Glauber approximation below the data points in Figs. 3 and 4 as the energy decreases below ~30 eV. At such low energies, where the whole idea of approximating the incident electron trajectory by a straight-line path breaks down, it is not easy to decide quantitatively what kinds of errors the Glauber approximation is producing; but it does seem that under these circumstances, supposing that $\vec{q}$ lies wholly in a single x, y plane perpendicular to the entire incident electron trajectory, whether this plane is supposed $\perp$ to $\vec{K}_i$ or to $\frac{1}{2}(\vec{K}_i+\vec{K}_f)$, makes the integral (1) an underestimate of the true $F_{fi}(\vec{q})$. This assertion is based on the effect of replacing q by $q_\perp<q$ in the expressions for $|F_{fi}|^2$ we have obtained [e.g., in Eq. (18)]; Fig. 8 shows that this replacement increases $|F_{fi}|^2$ at every angle. Actually, this unjustified simple replacement of q by $q_\perp$ is too crude, and at low energies brings the Glauber predictions well above the experimental data in Figs. 3 and 4. Nevertheless, it now seems reasonable that even if electron exchange is negligible one should expect the Glauber formula (1) to yield too small inelastic cross sections at those low energies for which the assumptions $\vec{q}\cdot\vec{K}_i=0$ and $\vec{q}\cdot\frac{1}{2}(\vec{K}_f+\vec{K}_i)=0$ both fail in a nonnegligible range of angles near $\theta=0$. By way of numerical illustration, we note that for $1s$-$2p$ excitation at $E_i=30$ eV, the right-hand side of (34) is about 0.4 at 30°.

It has been pointed out in Sec. III C that $F_{fi}(\vec{q})$ is identically zero for excitation to the $2p$ $m=0$ level. One easily verifies that this result implies the polarization fraction P [Eq. (33)] of the Lyman-α radiation following $1s$-$2p$ excitation should equal -1 at all incident electron energies. This result must be wrong, and indeed is quite at odds with the observations of Ott *et al.*,[33] who find $P(E_i)$ decreases monotonically from about $+0.2$ to -0.1 in the energy range 20 eV $<E_i<$ 700 eV. Moreover, these observations[33] of $P(E_i)$ are fairly well fitted by FBA calculations in this same energy range. Because the FBA predictions have not taken into account fine-structure and hyperfine effect complications (which cannot be ignored[39]), and because the observations include the effects of cascading, it is possible that the agreement between the FBA and measured $P(E_i)$ really is not as good as it seems. Nevertheless, it is obvious that the Glauber approximation fails badly for the purpose of predicting $P(E_i)$. Since the Glauber approximation has otherwise been so successful, some comments concerning this failure to predict $P(E_i)$ certainly are in order.

Actually the reasons the Glauber approximation predicts $P(E_i)$ so poorly at energies as high as 700 eV are not wholly transparent to us; but it is clear that use of $\vec{K}_i$ as the z axis in our calculations [in Eq. (22), specifically] is the source of the difficulty. As we have explained, for any given fixed $\vec{q}$ our results for $\sum|F_{fi}(\vec{q}, m_f)|^2$ summed over all m_f should be valid at not exceedingly low energies, independent of the axis of quantization of the final bound-state wave functions. This invariance does not hold for any given individual $|F_{fi}(\vec{q}, m_f)|^2$, however. At not exceedingly low energies, therefore, it is possible that the ratio of the individual Glauber partial cross sections $\sigma_{2p,1s}(m_f)$ for excitation to $2p$ $m_f=0, \pm1$ quantized along $\vec{K}_i$ can be quite wrong, even though the sum of these partial cross sections is reasonably accurate at any given θ.

At very high energies, however, where the contribution to the total excitation cross section comes almost entirely from forward scattering so that there is essentially no distinction between quantizing along $\vec{K}_i$ and quantizing along $\frac{1}{2}(\vec{K}_i+\vec{K}_f)$, the Glauber approximation prediction of $P=-1$ should be correct (always neglecting fine structure, hyperfine structure, and cascading). In this limit, moreover, the Glauber approximation and the FBA predictions of P should coincide. This ultimate coincidence is implied by the claim in Sec. III C that FBA formulas[13] and numerical calculations[14] indicate the probability of $1s$-$2p$ $m=0$ excitation at high energies is negligible compared to the probability of $1s$-$2p$ $m=\pm1$ excitation, with the atomic wave functions quantized along $\vec{K}_i$.

We also can give an independent demonstration of the equivalence of the FBA and the Glauber approximation predictions of $P(E_i)$ in the limit $E_i\to\infty$, as follows: In FBA, quantizing along $\vec{q}$, only the $2p$ $m=0$ level can be excited. When this state makes a radiative transition to the $1s$ state, the angular distribution $Q(\vec{\nu})$ of the emitted radiation is proportional[40] to $\sin^2\psi$, where ψ is the angle between $\vec{q}$ and $\vec{\nu}$, the direction of the outgoing radiation. So

$$Q(\vec{\nu})\sim 1-\cos^2\psi = 1-[\cos^2\theta_q\cos^2\theta_\nu + \sin^2\theta_q\sin^2\theta_\nu\cos^2(\phi_q-\phi_\nu)$$

$$+2\sin\theta_q \sin\theta_\nu \cos\theta_q \cos\theta_\nu \cos(\phi_q - \phi_\nu)], \quad (35)$$

where the angles θ_q, θ_ν, etc., are being specified relative to $\vec{K}_i$ as polar axis. Averaging (35) over the azimuth of $\vec{q}$, for fixed $\vec{\nu}$, we have

$$\langle Q(\vec{\nu})\rangle \sim 1 - \cos^2\theta_q \cos^2\theta_\nu - \tfrac{1}{2}\sin^2\theta_q \sin^2\theta_\nu . \quad (36)$$

Now at high energies and small scattering angles, the predominant contribution to the excitation is coming from $\vec{q}\perp\vec{K}_i$, as has been explained. So in this limit (36) reduces to

$$\langle Q(\vec{\nu})\rangle \sim 1 - \tfrac{1}{2}\sin^2\theta_\nu = \tfrac{1}{2}(1 + \cos^2\theta_\nu), \quad (37)$$

which is precisely the angular distribution of the radiation one infers[40] for transitions from $2p$ $m = \pm 1$ to $1s$, with no original occupation of the state $2p$ $m = 0$. Because it is known[21,33] that the angular distribution $Q(\vec{\nu})$ is uniquely related to the polarization fraction P, we now can conclude that for radiation following $1s$-$2p$ excitation the FBA and the Glauber P both equal -1 in the high-energy limit.

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