NASA TECHNICAL NOTE

NASA TN D-2903

COMPARISON OF GRYZINSKI'S AND BORN'S APPROXIMATIONS FOR INELASTIC SCATTERING IN ATOMIC HYDROGEN

by Carl F. Monnin and George M. Prok

Lewis Research Center
Cleveland, Ohio

COMPARISON OF GRYZINSKI'S AND BORN'S APPROXIMATIONS

FOR INELASTIC SCATTERING IN ATOMIC HYDROGEN

By Carl F. Monnin and George M. Prok

Lewis Research Center
Cleveland, Ohio

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

COMPARISON OF GRYZINSKI'S AND BORN'S APPROXIMATIONS FOR

INELASTIC SCATTERING IN ATOMIC HYDROGEN

by Carl F. Monnin and George M. Prok

Lewis Research Center

SUMMARY

Excitation cross sections for electron scattering in atomic hydrogen were determined by the Born approximation from the ground state to all excited states up to the 4f level. Gryzinski's semiclassical theory was used to obtain similar cross sections. Because of the small differences in energy between various energy levels of a principal quantum level, however, only the sum of cross sections for all transitions to the principal quantum level can be determined. Results of this method were compared with the sum of the individual sublevel cross sections determined by the Born approximation. Cross sections are presented for transitions from the ground state to n = 2, 3, 4, and ionization. The theoretical cross sections are compared with the experiment for the 1s → 2s, 1s → 2p, and 1s → ionization transitions. In addition, calculations of Gryzinski's electron exchange cross section were performed for the 2s, 3s, and 4s levels. Gryzinski's theory gave lower excitation cross sections than Born's approximation for all transitions up to n = 4 and for ionization. In the energy range considered (threshold to 360 eV), the cross sections resulting from the two theories are quite similar in shape and differ at various electron energies by a factor between 2 and 4. The exchange cross section of Gryzinski agrees very well with experiment for the 1s → 2s transition below 40 electron volts.

INTRODUCTION

One of the major energy loss mechanisms for a hot plasma is radiation. To predict the magnitude of this energy loss, a detailed knowledge of the cross sections involved is necessary. Hydrogen plasmas are of major importance for many research programs. For such plasmas, radiation losses are contributed by both the molecule and the atom constituents. The present investigation will concern itself only with atomic hydrogen cross sections.

Atomic hydrogen, the simplest atom, is attractive for theoretical studies of inelastic scattering by electron impact. Since atomic hydrogen readily recombines to form molecular hydrogen, its cross sections are difficult to obtain experimentally. Only the cross sections for the 1s → 2s, 1s → 2p, and 1s → ionization transitions have been measured (refs. 1 to 4). Most of the theoretical inelastic scattering calculations for atomic hydrogen cross sections have also been for these transitions (refs. 3 to 10). In the present investigation, cross sections for all hydrogen atom transitions from the ground state to the fourth quantum level and for ionization are presented for incident electron energies from threshold to 360 electron volts.

Two methods of calculating the pertinent cross sections are the Born approximation and the semiclassical theory of Gryzinski (refs. 11 and 12). The Born approximation is known to give valid results at high energies (ref. 13, p. 124). This fact permits normalization of experimental results to the Born approximation at energies above 200 electron volts (refs. 1 to 4). Gryzinski's semiclassical approach, on the other hand, agrees more closely with experiments in the low energy range (refs. 8 to 12 and 14). In this report, results obtained from the two theories are compared with each other and with some experimentally measured cross sections.

SYMBOLS

A	defined by eq. (A21)
a_0	Bohr radius, 5.29×10^{-9} cm
b	$\dfrac{(n + 1) - (n - 1)u}{2(1 - u)}$
$C_{n-\ell-1}^{\ell+2}(X)$	Gegenbauer polynomial defined by eq. (12)
E	energy loss of incident electron
E_1	kinetic energy of bound electron
E_2	kinetic energy of incident electron
e	electronic charge
$_2F_1$	hypergeometric function
g_e	defined by eq. (2)
g_j	defined by eq. (4)
h	Planck's constant, 6.6256×10^{-27} (erg)(sec)
$I_{0n}(K)$	Born's differential cross section, eq. (6)

I_r	defined by eq. (A11)
I_θ	defined by eq. (A10)
I_φ	defined by eq. (A6)
$J_s(t)$	Bessel function of first kind of order s and argument t
K	magnitude of momentum change
K_{max}	maximum momentum change, $k + k_{0n}$
K_{min}	minimum momentum change, $k - k_{0n}$
$\vec{K}$	momentum change
k	wave number of incident electron
k_{0n}	wave number of scattered electron
ℓ	orbital angular momentum quantum number
m	magnetic quantum number
$N_{n\ell m}$	normalizing factor defined by eq. (A4)
n	principal quantum number
$P_\ell^m(\cos\theta)$	Legendre polynomial
$Q(U_n)$	excitation cross section (Gryzinski theory)
$Q_e(U_n)$	exchange cross section
$Q_{0n}(K)$	excitation cross section (Born approximation)
R	radius vector of incident electron
r, θ, φ	spherical coordinates
$\vec{r}$	radius vector of bound electron
s, p, d, f	energy levels for $\ell = 0, 1, 2, 3$, respectively
U_i	ionization potential
U_n	energy of level n
u	dummy variable
$V(r, R)$	Coulomb potential between incident electron and an atom
v	defined by eq. (A19)
v_e	speed of incident electron
X	defined by eq. (10)

$\hat{y}_0$	unit vector in direction of incident electron
$\hat{y}_1$	unit vector in direction of scattered electron
Z	Kr
α	dummy subscript
β	dummy subscript
Γ	gamma function
γ	$1/2$
$\epsilon_{n\ell m}(K)$	defined by eq. (9)
ζ	$Kna_0/2$
μ	$\ell + 5/2$
ν	$\ell + 1/2$
ξ	$2r/na_0$
σ_0	6.53×10^{-14} cm^2 eV^2
$d\tau_R$	differential volume element in coordinate space of incident electron
$d\tau_r$	differential volume element in coordinate space of atomic electron
Ψ_n^*	excited state wave function
Ψ_0	ground state wave function
ω	given in eq. (A19)

THEORY

Cross sections for inelastic scattering of electrons by atomic hydrogen can be calculated in a number of ways. The methods investigated in this report are Gryzinski's semiclassical theory and Born's approximation.

Semiclassical (Gryzinski) Theory

Using a semiclassical approach, Gryzinski developed a theory giving excitation cross sections (refs. 11 and 12) and exchange cross sections (ref. 12). In this theory, s → s transitions are assumed to take place only by an electron exchange process. The cross section for this process is given by

4

$$Q_e(U_n) = \frac{\sigma_0}{U_n^2} \frac{U_{n+1} - U_n}{U_n} g_e\left(\frac{U_i}{U_n}; \frac{U_i}{U_{n+1}}; \frac{E_2 + U_i}{U_n}\right) \tag{1}$$

where

$$g_e\left(\frac{U_i}{U_n}; \frac{U_i}{U_{n+1}}; \frac{E_2 + U_i}{U_n}\right) = \left[\frac{U_n^2}{(E_2 + U_i)(E_2 + U_i - U_n)}\right] \begin{cases} \dfrac{U_n}{E_2 + U_i - U_{n+1}} & \text{if } U_{n+1} \leq E_2 \\[4mm] \dfrac{U_n}{U_i} \dfrac{E_2 - U_n}{U_{n+1} - U_n} & \text{if } U_{n+1} \geq E_2 \end{cases}$$

$$\tag{2}$$

According to Gryzinski's model, all transitions other than $s \rightarrow s$ transitions take place by an excitation process. Excitation cross sections are given by

$$Q(U_n) = \frac{\sigma_0}{U_n^2} g_j\left(\frac{E_2}{U_n}; \frac{E_1}{U_n}\right) \tag{3}$$

where

$$g_j\left(\frac{E_2}{U_n}; \frac{E_1}{U_n}\right) = \left(\frac{E_2}{E_1 + E_2}\right)^{3/2}$$

$$\begin{cases} \dfrac{2}{3}\dfrac{E_1}{E_2} + \dfrac{U_n}{E_2}\left(1 - \dfrac{E_1}{E_2}\right) - \left(\dfrac{U_n}{E_2}\right)^2 & \text{if } U_n + E_1 \leq E_2 \\[5mm] \dfrac{2}{3}\left[\dfrac{E_1}{E_2} + \dfrac{U_n}{E_2}\left(1 - \dfrac{E_1}{E_2}\right) - \left(\dfrac{U_n}{E_2}\right)^2\right]\left[\left(1 + \dfrac{U_n}{E_1}\right)\left(1 - \dfrac{U_n}{E_2}\right)\right]^{1/2} & \text{if } U_n + E_1 \geq E_2 \end{cases}$$

$$\tag{4}$$

and

$$\sigma_0 = 6.53 \times 10^{-14} \text{ cm}^2 \text{ eV}^2$$

In equations (1) to (4) U_n and U_{n+1} are the energies of the n and n + 1 levels. The ionization potential is U_i, and E_1 and E_2 are the kinetic energies of the bound and the incident electrons, respectively.

The excitation cross section $Q(U_n)$ is proportional to the probability that the incident electron will lose an amount of energy equal to or greater than the energy of the n level. Thus, the cross section for a given transition with loss of energy in the interval $U_n \leq E < U_{n+1}$ is given by

$$Q(U_n, U_{n+1}) = Q(U_n) - Q(U_{n+1}) \tag{5}$$

Since to excite the n + 1 level an amount of energy greater than or equal to U_{n+1} must be lost, equation (5) is just the cross section for exciting the n level.

For atomic hydrogen the sublevels of a given principal quantum level are separated by a small amount of energy, and the Gryzinski approach does not give meaningful results for individual transitions. An example is the n = 2 level of atomic hydrogen, which has one 2s level and two 2p levels separated by less than half a wave number. The 2s transition from the ground state can take place only by an electron exchange process in Gryzinski's theory, while the two 2p transitions occur by an excitation process. Agreement with experiment and the Born approximation was obtained when all the energy levels, except the s level, of a principal quantum level were averaged to determine an energy for the principal quantum level. This energy was used to determine an excitation cross section from the ground state to the principal quantum level. Since the Gryzinski method gives only one cross section for excitation to any principal quantum level, it is necessary to add all the Born approximation cross sections of the sublevels for that principal quantum level for comparison. The Born approximation cross section to the s level is not included, since it is not considered in Gryzinski's excitation cross section.

Born Approximation

For fast electrons ($v_e >> e^2/h$), the first Born approximation is sufficient to determine the excitation cross section of an atom. The differential cross section for excitation from the ground state to some excited state n with momentum change between K and K + dK is given by reference 13 as

$$I_{0n}(K)dK = \frac{8\pi^3 m^2}{h^4} \frac{K\,dK}{k^2} \left| \iint V(\vec{r}, \vec{R}) e^{i\vec{K}\cdot\vec{R}} \Psi_0(\vec{r}) \Psi_n^*(\vec{r}) d\tau_r\, d\tau_R \right|^2 \tag{6}$$

where the magnitude of the momentum change is given by

$$K = \left| k_{0n} \hat{y}_1 - k \hat{y}_0 \right| \tag{7}$$

in which $\frac{kh}{2\pi} \hat{y}_0$ and $k_{0n} \frac{h}{2\pi} \hat{y}_1$ are the initial and final momentum vectors of the scattered electron, respectively. The ground state and excited state wave functions of the atom are Ψ_0 and Ψ_n^*, respectively, and $V(\vec{r}, \vec{R})$ is the Coulomb potential between the incident electron and the atom. The differential volume elements in the coordinate space of the atomic and incident electrons are $d\tau_r$ and $d\tau_R$, respectively.

The indicated integration given in appendix[1] for atomic hydrogen gives

$$I_{0n}(K)dK = \frac{128\pi^5 m^2 e^4}{k^2 h^4} \frac{dK}{K^3} \left| \epsilon_{n\ell m}(K) \right|^2 \tag{8}$$

where

$$\epsilon_{n\ell m}(K) = 2^{2\ell+3} n^{\ell+1} (2\ell+1)^{1/2} (\ell+1)! \left[(n-\ell-1)!\right]^{1/2} \left[(n+\ell)!\right]^{-1/2}$$

$$(Ka_0)^\ell \frac{\left[(n-1)^2 + 4\zeta^2\right]^{(n-\ell-3)/2}}{\left[(n+1)^2 + 4\zeta^2\right]^{(n+\ell+3)/2}} \left\{ (n+1)\left[(n-1)^2 + 4\zeta^2\right] C_{n-\ell-1}^{\ell+2}(X) \right.$$

$$- 2n\left[(n-1)^2 + 4\zeta^2\right]^{1/2} \left[(n+1)^2 + 4\zeta^2\right]^{1/2} C_{n-\ell-2}^{\ell+2}(X)$$

$$\left. + (n-1)\left[(n+1)^2 + 4\zeta^2\right] C_{n-\ell-3}^{\ell+2}(X) \right\} \tag{9}$$

$$X \equiv (n^2 - 1 + 4\zeta^2) \left\{ \left[(n+1)^2 + 4\zeta^2\right]\left[(n-1)^2 + 4\zeta^2\right] \right\}^{-1/2} \tag{10}$$

---

[1] The correct evaluation of the integral in eq. (6) is given in ref. 13. Ref. 15 contains an additional factor, $\left[P_\ell^m(k - k_{0n} \cos\theta/K)\right]^2$, which should not be there. The discrepancy is due to the orientation of coordinates; the proper orientation yields the answer given in ref. 13 and the appendix of this report.

$$\zeta \equiv \frac{Kna_0}{2} \tag{11}$$

$$\sum_{n-\ell-1=0}^{\infty} C_{n-\ell-1}^{\ell+2}(X)u^{n-\ell-1} \equiv (1 - 2uX + u^2)^{-(\ell+2)} \tag{12}$$

To obtain the total cross section for a transition, integration over the limits of allowed momentum change must be performed; thus,

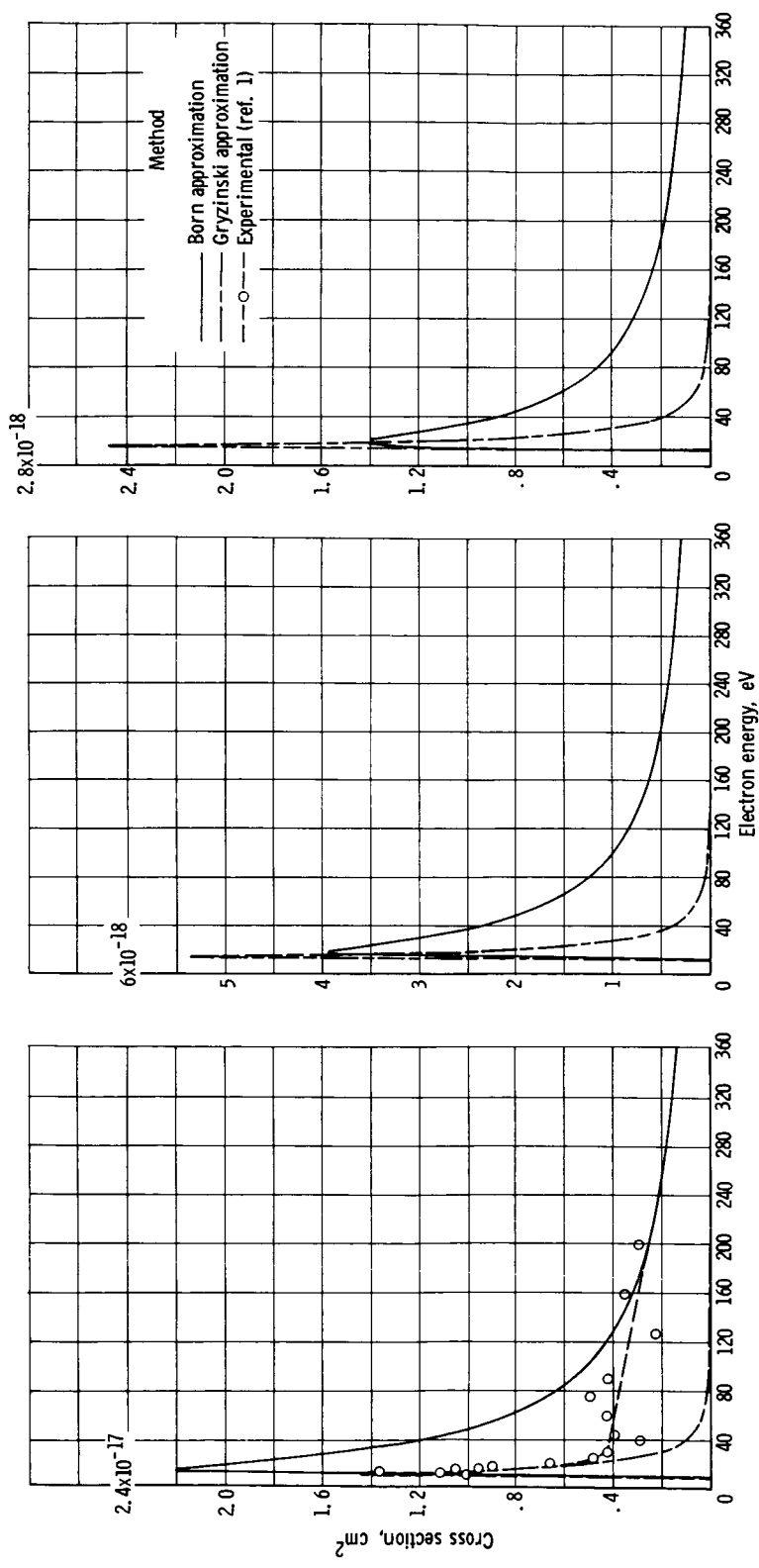$$Q_{0n}(K) = \int_{K_{min}}^{K_{max}} I_{0n}(K)dK \tag{13}$$

where

$$K_{max} = k + k_{0n}$$

$$K_{min} = k - k_{0n}$$

RESULTS AND DISCUSSION

The calculated results for the $1s \to ns$ transitions are shown in figures 1(a) to (c). The experimental results of Stebbings, et al., (ref. 1) for the $1s \to 2s$ transition are also shown in figure 1(a). Below 40 electron volts, Gryzinski's approximation yields cross sections which fit the experimental results very well. Since for the $1s \to ns$ transitions the Born approximation involves an excitation process whereas the Gryzinski approximation assumes an exchange process, it is not surprising that the results from the two methods do not agree.

The Born approximation results for the $1s \to np$, $1s \to nd$, and $1s \to nf$ transitions are shown in figures 2, 3, and 4, respectively. In addition, a composite cross section for excitation from the ground state to all sublevels of a principal quantum level was calculated using the Gryzinski model. The results are compared in figures 2(a), 5, and 6 (p. 10 to 12) with composite values obtained from the Born approximation by summing the sublevel cross sections. Experimental results for the $1s \to 2p$ transition from reference 2 are also included in figure 2(a); these results were normalized to the Born approximation at 200 electron volts. Finally, in figure 7 (p. 12), the Born approximation and the
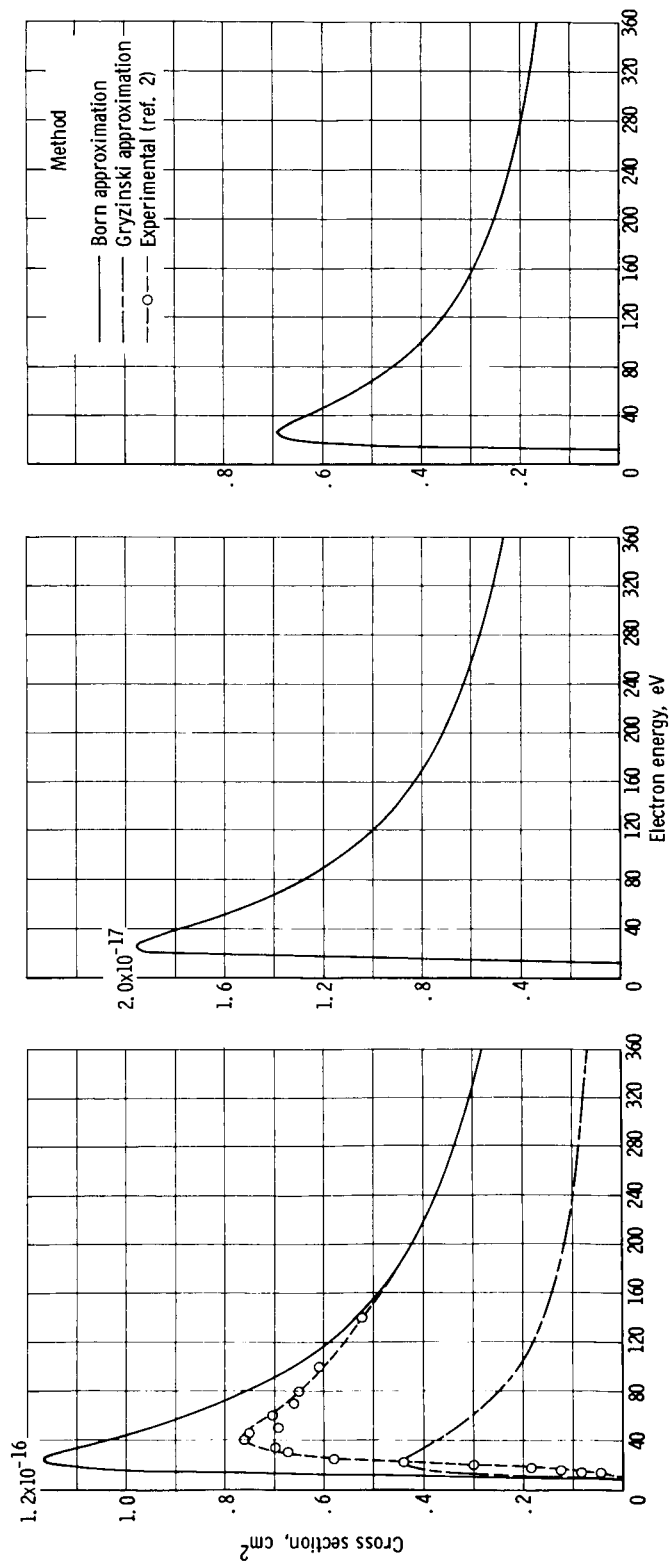
Method

——— Born approximation
— — Gryzinski approximation
— –o— Experimental (ref. 1)

2.8×10^{-18}

2.4

2.0

1.6

1.2

.8

.4

0

(c) Transition, 1s → 4s.

6×10^{-18}

5

4

3

2

1

0

(b) Transition, 1s → 3s.

Electron energy, eV

2.4×10^{-17}

2.0

1.6

1.2

.8

.4

0

Cross section, cm²

(a) Transition, 1s → 2s.

0 40 80 120 160 200 240 280 320 360

Figure 1. - Atomic hydrogen cross section for 1s → ns transitions.

(a) Transition, 1s → 2p.

(b) Transition, 1s → 3p.

(c) Transition, 1s → 4p.

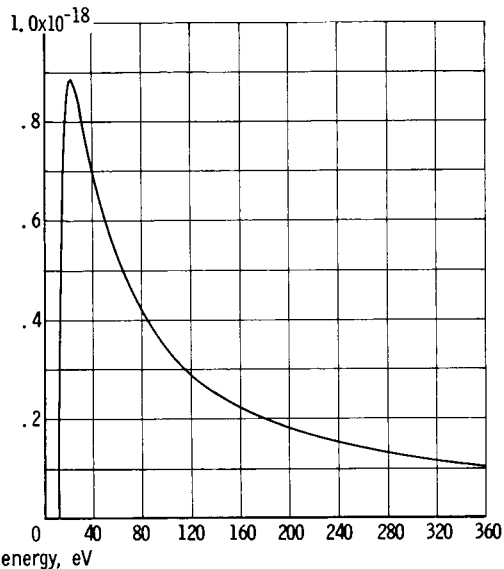Figure 2. - Atomic hydrogen cross section for 1s → np transitions.
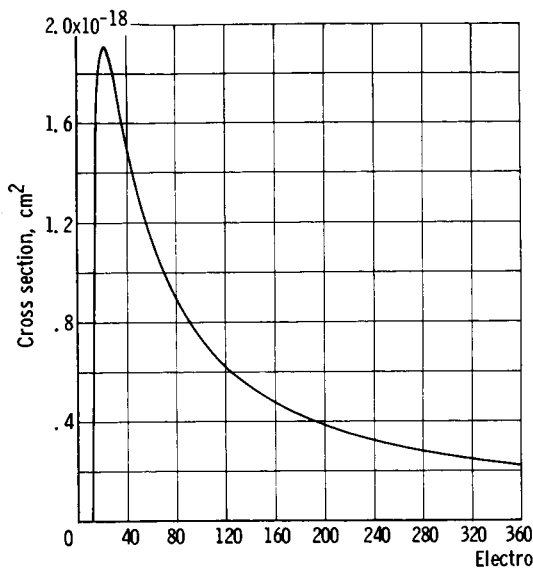
(a) Transition, 1s → 3d.

(b) Transition, 1s → 4d.

Figure 3. - Born approximation of atomic hydrogen cross section for 1s → nd transitions.

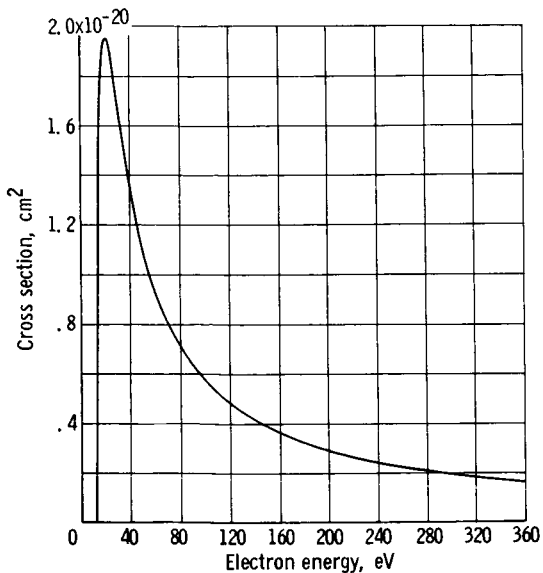Figure 4. - Born approximation of atomic hydrogen cross section for 1s → 4f transition.
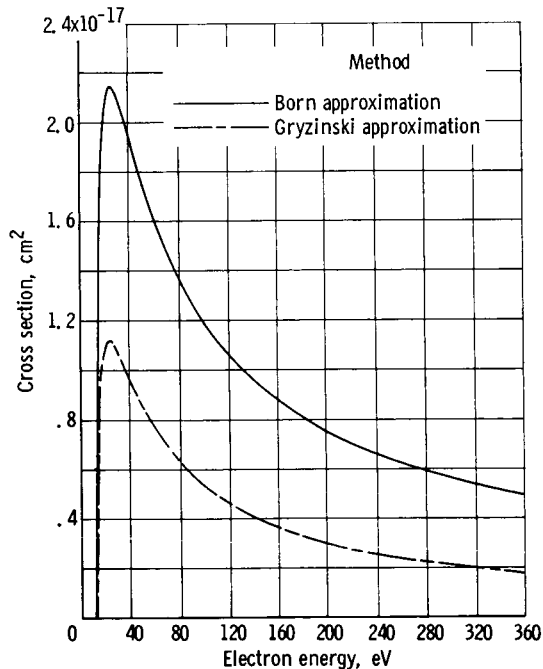

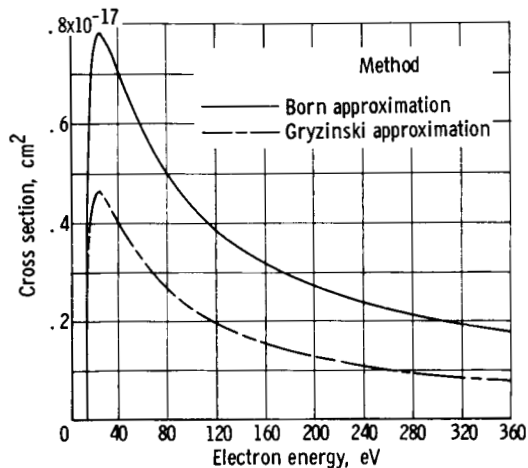
Figure 5. - Atomic hydrogen cross section for 1s → (3p + 3d) transition.

Figure 6. - Atomic hydrogen cross section for
1s → (4p + 4d + 4f) transition.

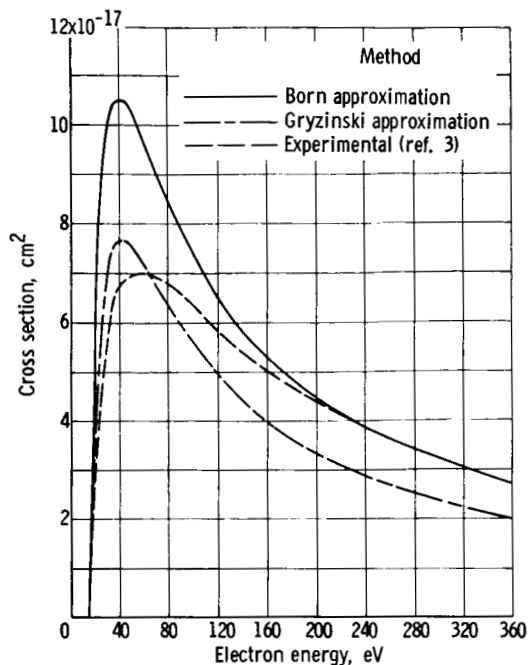Figure 7. - Atomic hydrogen cross section for
1s → ionization transition.

absolute experimental results reported in reference 3 for the 1s → ionization cross
section are compared with the results obtained by using Gryzinski's theory.

Semiclassical results for the 1s → 2p transition have been obtained by others
(refs. 6 to 8, 12, and 14), but the calculations were not carried to as high an energy as
those reported herein. The results reported herein for this transition agree with those
of references 8, 12, and 14, but they are about a factor of 2 less than those in refer-
ences 6 and 7. In reference 6, Saraph presents only the results of his calculations, and
thus it is impossible to determine why his results differ. Kingston (ref. 7) did not use
the exact Gryzinski model, and therefore, his results should not be expected to agree,
but they agree better with experimental results than the results reported herein.

Comparison of the results of the Gryzinski method and the Born approximation with
the experimental results of Fite and Brackmann (ref. 2) for the 1s - 2p transition
(fig. 2(a), p. 10) shows the maximum value of the experimental cross section to be about
half way between the maximum values of the two approximations. The experimental
maximum occurs at about twice the energy predicted by the two approximations.

Examination of figures 2(a) and 5 to 7 shows that as the principal quantum number
increases the percent difference between the two approximations decreases. As shown
in figure 2(a), the 1s → 2p transition at an electron energy of 360 electron volts is
found by the Gryzinski approximation to have a cross section about 24 percent of that
obtained by the Born approximation. For the 1s → ionization transition (fig. 7), the
Gryzinski cross section is about 75 percent of the Born cross section.

12

CONCLUDING REMARKS

Gryzinski's electron exchange model gives results in good agreement with experimental data for the 1s → 2s transition at electron energies below 40 electron volts. At higher energies, the electron exchange process contributes very little to the transition; the calculated cross sections become much smaller than the experimental ones.

In calculating composite cross sections for the excitation of atomic hydrogen to various principal quantum levels, Gryzinski's approximation gives values lower than those of the Born approximation although the shapes of the two curves are nearly the same. The difference between the two approximations becomes less as the principal quantum number increases.

For the 1s → ionization cross section, Gryzinski's method agrees well with the experimental absolute cross section. Except at low energies, where Gryzinski's theory predicts values higher than those determined by experiment, Gryzinski's theory gives results lower than the result of either the Born approximation or the experiment.

Lewis Research Center,
    National Aeronautics and Space Administration,
        Cleveland, Ohio, May 3, 1965.

APPENDIX - INTEGRATION OF EQUATION (6)

The integral to be evaluated is

$$I_{0n}(K)dK = \frac{8\pi^3 m^2}{h^4} \frac{K\, dK}{k^2} \left| \iint V(\vec{r}, \vec{R})e^{i\vec{K}\cdot\vec{R}}\Psi_0(\vec{r})\Psi_n^*(\vec{r})d\tau_r\, d\tau_R \right|^2 \tag{6}$$

where the potential $V(\vec{r}, \vec{R})$ is the Coulomb interaction between the incident and the atomic electrons $e^2/|\vec{r} - \vec{R}|$. The Coulomb interaction between the incident electron and the atomic nucleus e^2/R vanishes because of the orthogonality of the atomic wave functions.

Integration over the coordinate space of the incident electron by a method outlined in reference 16 yields

$$\int \frac{e^2}{|\vec{r} - \vec{R}|} e^{i\vec{K}\cdot\vec{R}}\, d\tau_R = \frac{4\pi}{K^2} e^2 e^{i\vec{K}\cdot\vec{r}} \tag{A1}$$

Substitution of equation (A1) into equation (6) gives

$$I_{0n}(K)dK = \frac{128\pi^5 m^2 e^4}{k^2 h^4} \frac{dK}{K^3} \left| \int e^{i\vec{K}\cdot\vec{r}}\Psi_0(\vec{r})\Psi_n^*(\vec{r})d\tau_r \right|^2 \tag{A2}$$

In order to evaluate equation (A2), the wave functions must be expressed in the coordinate system of the bound electron. With spherical coordinates, the wave function of atomic hydrogen becomes

$$\Psi_n(\vec{r}) \equiv \Psi_{n\ell m}(\vec{r}) = N_{n\ell m} r^\ell L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right) e^{-r/na_0} P_\ell^m(\cos\theta)e^{\pm im\varphi} \tag{A3}$$

where $N_{n\ell m}$ is a normalizing factor given by

$$N_{n\ell m}^2 = \frac{2^{2\ell}(2\ell + 1)(\ell - |m|)!\,(n - \ell - 1)!}{n\pi(na_0)^{2\ell+3}(\ell + |m|)!\,[(n + \ell)!]^3} \tag{A4}$$

Thus, the integral in equation (A2) becomes

14

$$\int e^{i\vec{K}\cdot\vec{r}}\Psi_{100}(\vec{r})\Psi_{n\ell m}(\vec{r})d\tau_r = N_{100}N_{n\ell m}\int_0^\infty \int_0^\pi \int_0^{2\pi} e^{i\vec{K}\cdot\vec{r}}e^{-r/a_0}$$

$$r^\ell L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right)e^{-r/na_0}P_\ell^m(\cos\theta)e^{\pm im\varphi}r^2\sin\theta\ d\varphi\ d\theta\ dr \qquad (A5)$$

If the Z-axis is alined along $\vec{K}$, the only contribution to the integral over φ is the exponential. Since the magnetic quantum number m is an integer,

$$I_\varphi = \int_0^{2\pi} e^{\pm im\varphi}\ d\varphi = \begin{cases} 0 & \text{for } m \neq 0 \\ \\ 2\pi & \text{for } m = 0 \end{cases} \qquad (A6)$$

The integral over θ is

$$I_\theta = \int_0^\pi e^{iKr\cos\theta}P_\ell(\cos\theta)\sin\theta\ d\theta \qquad (A7)$$

The Legendre polynomial (ref. 17, p. 77) can be expressed as a Gegenbauer polynomial in the form

$$P_\ell(\cos\theta) = C_\ell^{1/2}(\cos\theta) \qquad (A8)$$

Let $Z = Kr$ and $\nu = 1/2$, to put equation (A7) in the form of reference 17, page 77:

$$\int_0^\pi e^{iZ\cos\theta}C_\ell^\nu(\cos\theta)\sin^{2\nu}\theta\ d\theta = \frac{2^\nu\Gamma\left(\nu+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(2\nu+\ell)}{\ell!\,(2\nu)}i^\ell\frac{J_{\nu+\ell}(Z)}{Z^\nu} \qquad (A9)$$

If the form of equation (A9) is used, equation (A7) becomes

$$I_\theta = \left(\frac{2\pi}{Kr}\right)^{1/2}i^\ell J_{\ell+1/2}(Kr) \qquad (A10)$$

Incorporation of the terms involving r from equations (A5) and (A10) gives

15

$$I_r = \int_0^\infty e^{-r/a_0} r^\ell L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right) e^{-r/na_0} J_{\ell+1/2}(Kr) r^{3/2}\, dr \tag{A11}$$

Let

$$\xi = \frac{2r}{na_0}$$

and

$$\zeta = \frac{Kna_0}{2}$$

to put equation (A11) in the form

$$I_r = \left(\frac{na_0}{2}\right)^{\ell+5/2} \int_0^\infty e^{-(1+n)\xi/2} \xi^{\ell+3/2} L_{n+\ell}^{2\ell+1}(\xi) J_{\ell+1/2}(\xi\zeta)\, d\xi \tag{A12}$$

The Laguerre polynomial has a generating function (ref. 18, p. 784), which after differentiation α times with respect to ξ becomes

$$\sum_{\beta=0}^\infty \frac{L_{\alpha+\beta}^\alpha(\xi) u^\beta}{(\alpha+\beta)!} = \frac{(-1)^\alpha e^{-\xi \frac{u}{1-u}}}{(1-u)^{\alpha+1}} \tag{A13}$$

Employment of equation (A13) in equation (A12) gives

$$\sum_{n=\ell+1}^\infty \frac{I_r u^{n-\ell-1}}{(n+\ell)!} = -\left(\frac{na_0}{2}\right)^{\ell+5/2} \frac{1}{(1-u)^{2\ell+2}} \int_0^\infty e^{-\frac{[(n+1)-(n-1)u]\xi}{2(1-u)}} J_{\ell+1/2}(\xi\zeta) \xi^{\ell+3/2}\, d\xi$$

$$\tag{A14}$$

16

Let

$$b = \frac{(n + 1) - (n - 1)u}{2(1 - u)}$$

$$\nu = \ell + \frac{1}{2}$$

$$\mu = \ell + \frac{5}{2}$$

to put equation (A14) in the form of reference 16, page 32:

$$\int_0^\infty e^{-b\xi} J_\nu(\zeta\xi)\xi^{\mu-1} \, d\xi = \frac{\left(\frac{\zeta}{2b}\right)^\nu \Gamma(\mu+\nu)}{b^\mu \Gamma(\nu + 1)} \, {}_2F_1\left(\frac{\mu + \nu}{2}, \frac{\mu + \nu + 1}{2}; \nu + 1; -\frac{\zeta^2}{b^2}\right) \quad \text{(A15)}$$

which becomes

$$\sum_{n=\ell+1}^\infty \frac{I_r u^{n-\ell-1}}{(n + \ell)!} = \frac{-\left(\frac{na_0}{2}\right)^{\ell+5/2} \zeta^{\ell+1/2}(1 - u)2^{\ell+5/2}}{\left[(n + 1) - (n - 1)u\right]^{2\ell+3}} \frac{\Gamma(2\ell + 3)}{\Gamma\left(\ell + \frac{3}{2}\right)}$$

$$\quad {}_2F_1\left(\ell + \frac{3}{2}, \ell + 2; \ell + \frac{3}{2}; \frac{-4\zeta^2(1 - u)^2}{\left[(n + 1) - (n - 1)u\right]^2}\right) \quad \text{(A16)}$$

The hypergeometric series of equation (A16) can be expressed as

$${}_2F_1\left(\ell + \frac{3}{2}, \ell + 2; \ell + \frac{3}{2}; \frac{-4\zeta^2(1 - u)^2}{\left[(n + 1) - (n - 1)u\right]^2}\right) = \left\{1 + \frac{4\zeta^2(1 - u)^2}{\left[(n + 1) - (n - 1)u\right]^2}\right\}^{-\ell-2} \quad \text{(A17)}$$

Thus the integral over ξ becomes

$$\sum_{n=\ell+1}^{\infty} \frac{I_r u^{n-\ell-1}}{(n+\ell)!} = \frac{[(n+1) - (n-1)u](1-u)A}{(1 - 2Xv + v^2)^{\ell+2}} \qquad \text{(A18)}$$

where

$$v \equiv \omega u \equiv u \left[\frac{(n-1)^2 + 4\zeta^2}{(n+1)^2 + 4\zeta^2} \right]^{1/2} \qquad \text{(A19)}$$

$$X \equiv \frac{1}{\omega} \left[\frac{n^2 - 1 + 4\zeta^2}{(n+1)^2 + 4\zeta^2} \right] \qquad \text{(A20)}$$

$$A \equiv \frac{-2^{\ell+5/2} \zeta^{\ell+1/2} \Gamma(2\ell+3) \left(\dfrac{na_0}{2} \right)^{\ell+5/2}}{\left[(n+1)^2 + 4\zeta^2 \right]^{\ell+2} \Gamma\left(\ell + \dfrac{3}{2} \right)} \qquad \text{(A21)}$$

Equating coefficients of u gives

$$I_r = A(n+\ell)! \left[(n+1)\omega^{n-\ell-1} C_{n-\ell-1}^{\ell+2}(X) - 2n\omega^{n-\ell-2} C_{n-\ell-2}^{\ell+2}(X) + (n-1)\omega^{n-\ell-3} C_{n-\ell-3}^{\ell+2}(X) \right]$$

$$\text{(A22)}$$

where $C_{n-\ell-1}^{\ell+2}(X)$ is Gegenbauer's polynomial defined by

$$\sum_{n-\ell-1=0}^{\infty} C_{n-\ell-1}^{\ell+2}(X) u^{n-\ell-1} \equiv (1 - 2uX + u^2)^{-(\ell+2)} \qquad \text{(12)}$$

Addition of I_φ, I_θ, and I_r and substitution into equation (A5) yield

$$I_{0n}(K)dK = \frac{128\pi^5 m^2 e^4}{k^2 h^4} \frac{dK}{K^3} \left| \epsilon_{n\ell m}(K) \right|^2 \qquad \text{(8)}$$

18

where

$$\epsilon_{n\ell m}(K) = 2^{2\ell+3} n^{\ell+1} (2\ell+1)^{1/2} (\ell+1)! \left[(n-\ell-1)!\right]^{1/2} \left[(n+\ell)!\right]^{-1/2}$$

$$(Ka_0)^\ell \frac{\left[(n-1)^2 + 4\zeta^2\right]^{(n-\ell-3)/2}}{\left[(n+1)^2 + 4\zeta^2\right]^{(n+\ell+3)/2}} \left\{ (n+1)\left[(n-1)^2 + 4\zeta^2\right] C_{n-\ell-1}^{\ell+2}(X) \right.$$

$$- 2n\left[(n-1)^2 + 4\zeta^2\right]^{1/2} \left[(n+1)^2 + 4\zeta^2\right]^{1/2} C_{n-\ell-2}^{\ell+2}(X)$$

$$\left. + (n-1)\left[(n+1)^2 + 4\zeta^2\right] C_{n-\ell-3}^{\ell+2}(X) \right\} \tag{9}$$

REFERENCES

1. Stebbings, R. F.; Fite, Wade L.; Hummer, David G.; and Brackmann, R. T.: Collisions of Electrons with Hydrogen Atoms. V. Excitation of Metastable 2s Hydrogen Atoms. Phys. Rev., vol. 119, no. 6, Sept. 15, 1960, pp. 1939-1945.

2. Fite, Wade L.; and Brackmann, R. T.: Collisions of Electrons with Hydrogen Atoms. II. Excitation of Lyman-Alpha Radiation. Phys. Rev., vol. 112, no. 4, Nov. 15, 1958, pp. 1151-1156.

3. Bates, D. R., ed.: Atomic and Molecular Process. Academic Press, Inc., 1962.

4. Burke, P. G.; and Smith, Kenneth: The Low-Energy Scattering of Electrons and Positrons by Hydrogen Atoms. Rev. Mod. Phys., vol. 34, no. 3, July 1962, pp. 458-502.

5. Omidvar, Kazem: Theory of the 2s and 2p Excitation of the Hydrogen Atom Induced by Electron Impact. NASA TN D-2145, 1964.

6. Saraph, H. E.: Cross Sections for $n \rightarrow n+1$ Transitions in Hydrogen Produced by Electron Impact. Proc. Phys. Soc., vol. 83, May 1964, pp. 763-768.

7. Kingston, A. E.: Excitation and Ionization of Hydrogen Atoms by Electron Impact. Phys. Rev., vol. 135, no. 6A, Sept. 14, 1964, pp. 1529-1536.

8. Omidvar, Kazem: Excitation of the Hydrogen Atom by Electron Collision. NASA TM X-55082 (X-641-64-193), 1964.

9. Omidvar, Kazem: Ionization of the Hydrogen Atom by Electron Collision. NASA TM X-55081 (X-641-64-192), 1964.

10. McCarroll R.: The Excitation of the Discrete Levels of Atomic Hydrogen by Fast Electrons. Proc. Phys. Soc., ser. A, vol. 70, pt. 6, June 1957, pp. 460-465.

11. Gryzinski, Michal: Classical Theory of Electronic and Ionic Inelastic Collisions. Phys. Rev., vol. 115, no. 2, July 15, 1959, pp. 374-383.

12. Gryzinski, Michal: Classical Theory of Atomic Collisions. I. Inelastic Atomic Collisions. Rept. No. PAN-448/XVIII, Polish Acad. Sci., Inst. Nuclear Res. (Warsaw), June 1963.

13. Mott, N. F.; and Massey, H. S. W.: The Theory of Atomic Collisions. Second ed., Clarendon Press (Oxford), 1949.

14. Ochkur, V. I.; and Petrunkin, A. M.: The Classical Calculation of the Probabilities of Excitation and Ionization of Atoms by Electron Impact. Optics and Spectroscopy, vol. 14, no. 3, Mar. 1963, pp. 245-248.

15. Massey, H.S.W.; and Mohr, C.B.O.: The Collision of Electrons with Simple Atomic Systems and Electron Exchange. Proc. Roy. Soc. (London), ser. A, vol. 132, no. 820, Aug. 1, 1931, pp. 605-630.

16. Schiff, L.I.: Quantum Mechanics. Second ed., McGraw-Hill Book Co., Inc., 1955.

17. Magnus, W.; and Oberhettinger, F. (J. Wermer, trans.): Formulas and Theorems for the Functions of Mathematical Physics. Chelsea Pub. Co., Inc., 1949.

18. Morse, P.M.; and Feshbach, H.: Methods of Theoretical Physics. McGraw-Hill Book Co., Inc., 1953.