

X-641-64-192

TM X-55081

FACILITY FORM 802

N64-33633

(ACCESSION NUMBER)

(THRU)

(PAGES)

(CODE)

(NASA CR OR TMX OR AD NUMBER)

(CATEGORY)

# IONIZATION OF THE HYDROGEN ATOM BY ELECTRON COLLISION

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OTS PRICE

\$ 3,00FS  
\$ 75ME

XEROX

MICROFILM

JULY 1964



GODDARD SPACE FLIGHT CENTER

GREENBELT, MARYLAND

## SUMMARY

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By the use of the parabolic coordinate a general formula is derived for ionization of the hydrogen atom by electron collision when the atom is in any given initial state. Using this formula the total ionization cross section and the ionization cross section per unit energy range of the ejected electrons for all substates of the hydrogen atom belonging to the principal quantum numbers  $n = 1, 2, 3, 4, 5$  are tabulated. In addition the ionization cross section of one substate from each of the principal quantum numbers  $n = 6, 7, 8, 9, 10$  are tabulated. These tables cover the range of energies of interest in the plasma calculations. The approximation used is the Born approximation in which the bombarding electron before and after collision is described by a plane wave, and the ejected electron by a Coulomb wave function. Comparison with experiment for the ground state of the atom is given.

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## I. INTRODUCTION

Apart from purely theoretical interest, ionization is one of the main atomic processes in the stellar atmosphere. This process occurs also in gas discharges and in plasma. Of the two competing forms of ionization, photoionization and electron impact ionization, the photoionization cross section of any excited state of hydrogen is known with good accuracy; this, however, is not true of the electron impact ionization. It is then desirable to know the electron impact ionization when atoms are in highly excited states. Because of practical difficulties in the measurement of the ionization cross section of excited states, the corresponding calculation becomes more important.

We review briefly the developments of the theoretical and experimental works on this particular form of ionization. The classical value of the ionization cross section with the atom in any initial state has been calculated by J. J. Thomson<sup>1</sup> (1912). Massey and Mohr<sup>2</sup> (1933) have calculated, within the Born approximation, the ground state ionization of the hydrogen atom. Burhop<sup>3</sup> (1940), extending the same technique, formulated the ionization from substates of the first excited state without giving any numerical results for the case of hydrogen. B. Yavorsky<sup>4</sup> (1945) has given the ionization of all S states of hydrogen in a general way, in the form of a triple sum and triple integrations. The results for 2S and 3S states are shown in this paper graphically. Mandl<sup>5</sup> (1952), rederiving the equations of Burhop, has given the results of ionization from the 2P,  $M = \pm 1$  states, again in graphical form. Later

on Swan<sup>6</sup> (1955), taking the equations of Burhop, has carried out the numerical integrations which are tabulated for the 2S, 2P,  $M = 0, \pm 1$  states. Aside from a factor of 2, it will be shown later that his results seem not too accurate.

Outside of the Born approximation, Geltman<sup>7</sup> (1956) has considered the effect of the Coulomb field of the nucleus on the incident electron, an effect which is neglected in the Born approximation. This effect is obviously important at the threshold of ionization. He finds a law in which the cross section near threshold is proportional to the excess energy of the ionizing electron.

At this time the first measurement of the ionization of hydrogen became available. Fite and Brackmann<sup>8</sup> (1958) achieved this measurement and, without much surprise, showed that the measurement agrees with the Born approximation beyond 100 ev. This measurement was followed by those of Boyd and Boksenberg<sup>9</sup> (1959), and Rothe et al.<sup>10</sup> (1962).

The other theoretical works of interest include the inclusion of exchange in ionization by Peterkop<sup>11</sup> (1961), the ionization by the impulse approximation by Akerib and Borowitz<sup>12</sup> (1961), the ionization by close coupling approximation by Taylor and Burke<sup>13</sup> (1963), and the threshold law for ionizing collisions by Rudge and Seaton<sup>14</sup> (1964).

Returning to the Born approximation, this approximation consists in representing the ionizing electron in the quantum mechanical calculations by a plane wave, the bound electron by a hydrogenic wave function, and the ejected electron by a Coulomb wave function. Physically,

this is to say that, when the ionization takes place, the ionizing electron is far from the nucleus, so that only one electron is in the field of the nucleus. The approximation also consists of the exclusion of two less important effects: the exchange of the two electrons, and the effect of the polarization of the atom on the incident electron.

Application of the hydrogenic wave function in parabolic coordinates in the expression for the ionization amplitude facilitates its evaluation. This is because the final state in this expression, which is the eigenfunction of the ejected electron, is easily expressed in parabolic coordinates. In this paper generating function in parabolic coordinates is used to express in closed form the ionization amplitude involving an arbitrary initial state.

With the nucleus fixed, the total ionization cross section involves twelve integrals: six integrals over the spatial coordinates of the two electrons, and the next six over the momentum coordinates of the two electrons. For a given incident electron energy, the conservation of energy eliminates one integral.<sup>15</sup> Of the remaining eleven integrations, nine are carried out analytically, and two integrations—integrations with respect to the magnitudes of the momentum transfer of the incident electron, and the momentum of the ejected electron—are carried out numerically by a computer.

In the calculation that follows the cross section for a given  $n$  and a particular bound electron orbital angular momentum  $l$  is not available anymore, although this can be obtained by a unitary transformation of

the ionization amplitude before the integration is carried out to find the total cross section.

## II. FORMULATION

### Born Amplitude for Ionization and Excitation

Consider a system of an electron and a hydrogen atom in an arbitrary state. Collision of the electron with the atom may result in the excitation of the atom into a different state, or its ionization. Let  $\mathbf{k}_0$  represent the propagation vector of the electron before collision, and  $\mathbf{k}_1$  the same vector after collision; the equation for conservation of energy will be

$$E = E_0 + \frac{\hbar^2 k_0^2}{2m} = E_1 + \frac{\hbar^2 k_1^2}{2m}, \quad (1)$$

where  $E_0$  and  $E_1$  are the energies of the isolated atom before and after collision, and  $E$  is the total energy of the system. The Born excitation or ionization amplitude can then be written<sup>16, 17, 18</sup>

$$f(\theta_1, \phi_1) = \frac{2me^2}{4\pi\hbar^2} \int \exp[i(\mathbf{k}_0 - \mathbf{k}_1) \cdot \mathbf{r}_1] \psi_f^*(\mathbf{r}_2) \left( \frac{Z}{r_1} - \frac{1}{r_{12}} \right) \psi_i(\mathbf{r}_2) \times d^3\mathbf{r}_1 d^3\mathbf{r}_2. \quad (2)$$

In this equation  $\theta_1, \phi_1$  are the polar angles of  $\mathbf{k}_1$  with respect to  $\mathbf{k}_0$  as the  $z$ -axis,  $m$  and  $e$  are the electronic mass and charge,  $Z$  the charge number of the nucleus,  $\mathbf{r}_1$  and  $\mathbf{r}_2$  the position vectors of the incident and the atomic electrons,  $\psi_i(\mathbf{r}_2)$  and  $\psi_f(\mathbf{r}_2)$  the initial and the final eigenfunctions of the atom, and  $r_1$  and  $r_{12}$  the distances of the incident electron from the nucleus and the atomic electron, respectively. The probability that an incident electron, after causing the transition

specified by  $\psi_i$  and  $\psi_f$ , be scattered within a range of solid angles  $\omega_1$  to  $\omega_1 + d\omega_1$  is given by

$$I(\theta_1, \phi_1) d\omega_1 = \frac{k_1}{k_0} |f(\theta_1, \phi_1)|^2 d\omega_1, \quad (3)$$

where  $I(\theta_1, \phi_1)$  is the differential cross section. It is convenient to introduce the momentum transfer vector  $\mathbf{K}$  through

$$\mathbf{K} = \mathbf{k}_0 - \mathbf{k}_1. \quad (4)$$

Squaring and taking the differential with respect to  $\theta_1$  of this equation gives

$$K dK = k_0 k_1 \sin \theta_1 d\theta_1 = k_0 k_1 \frac{d\omega_1}{2\pi}; \quad (5)$$

the last equality follows from the axial symmetry of the problem. When equation (2) is substituted in equation (3) and note is taken of equation (5), the orthogonality of  $\psi_i$  and  $\psi_f$ , and the relation<sup>16</sup>

$$\int \frac{\exp [i \mathbf{K} \cdot \mathbf{r}_1]}{r_{12}} d^3 \mathbf{r}_1 = \frac{4\pi}{K^2} \exp [i \mathbf{K} \cdot \mathbf{r}_2], \quad (6)$$

we obtain

$$I(\mathbf{K}) dK = \frac{8\pi}{a_0^2 k_0^2} |V(\mathbf{K})|^2 \frac{dK}{K^3}, \quad (7)$$

$$V(\mathbf{k}) = \int \exp [i \mathbf{K} \cdot \mathbf{r}] \psi_i(\mathbf{r}) \psi_f^*(\mathbf{r}) d^3 \mathbf{r}. \quad (8)$$

In the above expression  $a_0$  is the Bohr radius, and the direction of the polar axis in the integral for  $V(\mathbf{K})$  is along  $\mathbf{K}$ ; while for the definition of  $f(\theta_1, \phi_1)$  the polar axis was taken along  $\mathbf{k}_0$ .

The total cross section for excitation is obtained by integrating the above expression over all possible values of  $\mathbf{K}$ :

$$Q_e = \frac{8\pi}{a_0^2 k_0^2} \int_{k_0 - k_1}^{k_0 + k_1} |V(\mathbf{K})|^2 \frac{d\mathbf{K}}{K^3}, \quad (9)$$

where the limits of integration are fixed by equation (4). In the case of ionization, in contrast to excitation, the ejected electron may occupy in the continuum any of the infinitely many energetically permissible states; while in the case of excitation the bound electron occupies a single final state. The cross section for ionization is obtained by integrating over all final states in addition to integration over  $\mathbf{K}$ . If  $\mathbf{k}$  is the propagation vector of the ejected electron with polar coordinates  $k, \theta_k, \phi_k$  in a coordinate system whose  $z$  axis is along  $\mathbf{K}$ , the ionization amplitude becomes a function of  $\mathbf{k}$  also. The cross section is then given by

$$\begin{aligned} Q_i &= \frac{8\pi}{a_0^2 k_0^2} \int |V(\mathbf{k}, \mathbf{K})|^2 \frac{d^3 \mathbf{k} d\mathbf{K}}{K^3} \\ &= \frac{8\pi}{a_0^2 k_0^2} \int_0^{k_{\max}} \int_{-1}^{+1} \int_0^{2\pi} \int_{k_0 - k_1}^{k_0 + k_1} |V(\mathbf{k}, \mathbf{K})|^2 \times \frac{k^2 dk dx d\phi_k d\mathbf{K}}{K^3}, \quad (10) \end{aligned}$$

when we have written

$$\cos \theta_k = x . \quad (11)$$

Let  $n$  be the principal quantum number of the atom before ionization;

substitution of  $E_0 = -\frac{Z^2 e^2}{2a_0 n^2}$ ,  $E_1 = \frac{\hbar^2 k^2}{2m}$  in equation (1) gives

$$k^2 + k_1^2 = k_0^2 - \frac{Z^2}{a_0^2 n^2} , \quad (12)$$

$$k_{\max}^2 = k_0^2 - \frac{Z^2}{a_0^2 n^2} . \quad (13)$$

### Use of the Generating Functions

To evaluate  $V$ , we have to specify the initial and the final states.

For the initial state we take the hydrogen eigenfunction in parabolic coordinates,<sup>19, 20</sup>

$$\phi_{n_1 n_2 m}(\xi, \eta, \phi) = N_{n_1 n_2 m} \exp\left[-\frac{1}{2} \alpha(\xi + \eta)\right] (\xi \eta)^{\frac{1}{2}m} \times L_{n_1+m}^m(\alpha \xi) L_{n_2+m}^m(\alpha \eta) \cos m\phi ;$$

$$\alpha = \frac{Z}{n} ; \quad n_1, n_2, m = 0, 1, 2, 3, \dots . \quad (14)$$

The arguments of these functions are related to the Cartesian and polar coordinates of the bound electron through

$$\left. \begin{aligned} x &= r \sin \theta \cos \phi = \sqrt{\xi \eta} \cos \phi , \\ y &= r \sin \theta \sin \phi = \sqrt{\xi \eta} \sin \phi , \\ z &= r \cos \theta = \frac{1}{2} (\xi - \eta) . \end{aligned} \right\} \quad (15)$$

The quantum numbers  $n_1, n_2, m$  are related to  $n$  by

$$n_1 + n_2 + m = n - 1, \quad (16)$$

so that there are three independent quantum numbers only, corresponding to the three degrees of freedom of the bound electron.  $n$  is the principal quantum number similar to spherical coordinates, while  $m$  is the absolute value of the magnetic quantum number defined in the latter coordinates. To fix the normalization constant  $N_{n_1 n_2 m}$ , we first find the element of volume in parabolic coordinates. If only  $\xi$  of the three orthogonal coordinates  $\xi, \eta, \phi$  is varied, the corresponding line element, with the help of equation (15), may be written

$$ds_\xi^2 = dx^2 + dy^2 + dz^2 = \left(\frac{\partial x}{\partial \xi}\right)^2 d\xi^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 d\xi^2 + \left(\frac{\partial z}{\partial \xi}\right)^2 d\xi^2 = \frac{\xi + \eta}{4\xi} d\xi^2.$$

Similarly,

$$ds_\eta^2 = \frac{\xi + \eta}{4\eta} d\eta^2, \quad ds_\phi^2 = \xi\eta d\phi^2.$$

Therefore,

$$dv = ds_\xi ds_\eta ds_\phi = \frac{1}{4} (\xi + \eta) d\xi d\eta d\phi. \quad (17)$$

$N_{n_1 n_2 m}$  is found through an orthogonality and a recurrence formula for the associated Laguerre polynomials,<sup>21</sup>

$$\int_0^\infty z^m e^{-z} L_{n+m}^m(z) L_{n'+m}^m(z) dz = \delta(n, n') \times \left[ \frac{(m+n)!}{n!} \right]^3, \quad (18)$$

$$zL_{n+m}^m(z) = (m+2n+1)L_{n+m}^m(z) - \frac{n+1}{m+n+1}L_{n+1+m}^m(z) - (m+n)^2L_{n-1+m}^m(z). \quad (19)$$

Normalization of equation (14), with the help of the last three equations, gives

$$N_{n_1 n_2 m} = \left(\frac{\epsilon_m}{2\pi}\right)^{1/2} \times \left(\frac{2}{n}\right)^{1/2} \times a^{m+3/2} \times \frac{[n_1! n_2!]^{1/2}}{[(n_1+m)! (n_2+m)!]^{3/2}}, \quad (20)$$

$$\epsilon_m = \begin{cases} 2, & m \neq 0 \\ 1, & m = 0 \end{cases}. \quad (21)$$

Equation (14) can be expressed as a linear combination of the hydrogenic eigenfunction in spherical polar coordinates, and the two representations are related through a unitary transformation. As an example,  $\phi_{100}$  and  $\phi_{010}$  are the two zeroth order eigenfunctions of the hydrogen atom in a weak external electric field, used in the first order Stark effect.

The final state in V should describe the ejected electron in the Coulomb field of the nucleus. Let us designate it by  $\psi(\mathbf{k}, \mathbf{r})$ ; then it is justified<sup>20,22</sup> to write

$$\psi(\mathbf{k}, \mathbf{r}) = e^{ikz} L(\eta), \quad (22)$$

where  $L(\eta)$  is a function of the parabolic coordinate  $\eta$  only. Substitution of equation (22) in the Schrödinger equation for  $\psi(\mathbf{k}, \mathbf{r})$  gives

$$\eta L'' + (1 - ik\eta) L' + \beta k L = 0, \quad \beta = \frac{Z}{ka_0}. \quad (23)$$

It can be verified, by direct differentiation, that a solution to the above differential equation is given by

$$L(\eta) = N e^{ik\eta} \int_0^{\infty} e^{-u} u^{-i\beta} J_0 [2\sqrt{iuk\eta}] du , \quad (24)$$

where  $J_0$  is the Bessel function of the zeroth order and  $N$  is the normalization constant whose value is given below and is found elsewhere<sup>23</sup>:

$$N = \frac{1}{2\pi} \left[ \frac{\beta}{1 - \exp(-2\pi\beta)} \right]^{1/2} \frac{1}{\Gamma(1 - i\beta)} . \quad (25)$$

Equation (22) can now be written

$$\begin{aligned} \psi(\mathbf{k}, \mathbf{r}) = & \frac{1}{2\pi} \left[ \frac{\beta}{1 - \exp(-2\pi\beta)} \right]^{1/2} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\Gamma(1 - i\beta)} \\ & \times \int_0^{\infty} e^{-u} u^{-i\beta} J_0 (R) du , \end{aligned} \quad (26)$$

where

$$R = 2 [iu(kr - \mathbf{k} \cdot \mathbf{r})]^{1/2} , \quad (27)$$

with the appropriate asymptotic form<sup>23</sup>

$$\psi(\mathbf{k}, \mathbf{r}) \sim (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}} . \quad (28)$$

Having fixed the initial and the final state in the matrix V, we proceed with its evaluation. By equation (15),

$$\begin{aligned} \mathbf{k} \cdot \mathbf{r} &= k \left[ r - x \sin \theta_k \cos \phi_k - y \sin \theta_k \sin \phi_k - z \cos \theta_k \right] \\ &= k \left[ \xi \sin^2 \frac{\theta_k}{2} + \eta \cos^2 \frac{\theta_k}{2} - 2\sqrt{\xi\eta} \sin \frac{\theta_k}{2} \cos \frac{\theta_k}{2} \cos (\phi - \phi_k) \right] ; \end{aligned}$$

then we can write

$$R^* = \left[ \rho^2 + \sigma^2 - 2\rho\sigma \cos (\phi - \phi_k) \right]^{1/2} , \quad (29)$$

where

$$\left. \begin{aligned} \rho &= 2\sqrt{-iuk} \sin \frac{\theta_k}{2} \sqrt{\xi} , \\ \sigma &= 2\sqrt{-iuk} \cos \frac{\theta_k}{2} \sqrt{\eta} . \end{aligned} \right\} \quad (30)$$

Equation (8) can now be written

$$\begin{aligned} V(\mathbf{k}, \mathbf{K}) &= \frac{N_{n_1 n_2 m}}{2\pi} \left( \frac{\beta}{1 - e^{-2\pi\beta}} \right)^{1/2} \frac{1}{4\Gamma(1 + i\beta)} \\ &\times \iiint \exp \left[ -\frac{1}{2} a(\xi + \eta) + \frac{i}{2} K(\xi - \eta) - \frac{i}{2} k(\xi + \eta) - u \right] \\ &\times (\xi\eta)^{m/2} L_{n_1+m}^m(a\xi) L_{n_2+m}^m(a\eta) \cos(m\phi) \\ &\times u^{i\beta} J_0(R^*) (\xi + \eta) du d\xi d\eta d\phi . \end{aligned} \quad (31)$$

We first carry the integration with respect to  $\phi$ . Aside from  $\cos(m\phi)$  the only term in the integrand of equation (31) which is a function of  $\phi$  is  $J_0(R^*)$ . By the addition theorem for the Bessel functions,<sup>24</sup>

$$J_0(R^*) = \sum_{n=0}^{\infty} \epsilon_n J_n(\rho) J_n(\sigma) \cos n(\phi - \phi_k) \quad , \quad (32)$$

where  $\epsilon_n$  is defined in (21), we get

$$\int_0^{2\pi} J_0(R^*) \cos m\phi d\phi = 2\pi J_m(\rho) J_m(\sigma) \cos m\phi_k \quad . \quad (33)$$

It is convenient to introduce the function  $I(m n_1 n_2 | k K \theta_k)$  by

$$V(k, K, \theta_k, \phi_k) = \frac{1}{2\pi} \left( \frac{\beta}{1 - e^{-2\pi\beta}} \right)^{1/2} \cos(m\phi_k) I(m n_1 n_2 | k K \theta_k) \quad ; \quad (34)$$

then, through equation (33),

$$\begin{aligned} I(m n_1 n_2 | k K \theta_k) &= \frac{\pi N_{n_1 n_2^m}}{2\Gamma(1+i\beta)} \times \iiint \exp \left[ -\frac{1}{2} (\alpha + ik) (\xi + \eta) + \frac{i}{2} K(\xi - \eta) - u \right] \\ &\quad \times (\xi\eta)^{m/2} \times L_{n_1+m}^m(\alpha\xi) L_{n_2+m}^m(\alpha\eta) u^{i\beta} \\ &\quad \times J_m(\rho) J_m(\sigma) (\xi + \eta) du d\xi d\eta \quad . \quad (35) \end{aligned}$$

The cross section, equation (10), can be expressed in terms of  $I(m n_1 n_2 | k K \theta_k)$  by integrating over  $\phi_k$ , changing now to atomic units

by putting  $a_0 = 1$ , and suppressing  $i$  for simplicity:

$$Q(n m n_1 n_2) = \frac{2Z}{\pi k_0^2} \left( \frac{2\pi}{\epsilon_m} \right) \int_0^{k_{\max}} \int_{k_0 - k_1}^{k_0 + k_1} \int_{-1}^{+1} |I(m n_1 n_2 | k K \theta_k)|^2 \times \frac{k dk dK dx}{K^3 (1 - e^{-2\pi Z/k})} \quad (36)$$

Below  $I(m n_1 n_2)$  is evaluated by means of the generating functions of the associated Laguerre polynomials. These are<sup>19</sup>

$$\left. \begin{aligned} \sum_{n_1=0}^{\infty} \frac{L_{n_1+m}^m(\alpha\xi)}{(n_1+m)!} s^{n_1+m} &= \frac{(-s)^m \exp\left[-\frac{\alpha\xi s}{1-s}\right]}{(1-s)^{m+1}}, \\ \sum_{n_2=0}^{\infty} \frac{L_{n_2+m}^m(\alpha\eta)}{(n_2+m)!} t^{n_2+m} &= \frac{(-t)^m \exp\left[-\frac{\alpha\eta t}{1-t}\right]}{(1-t)^{m+1}}. \end{aligned} \right\} (37)$$

If we introduce

$$p = \frac{\alpha}{2} + \frac{ik}{2}, \quad q = -\frac{iK}{2} \quad (38)$$

in equation (35), we see that

$$\begin{aligned}
\sum_{n_1, n_2} \frac{s^{n_1}}{(n_1 + m)!} \times \frac{t^{n_2}}{(n_2 + m)!} I(m, n_1, n_2) &= \frac{1}{(1-s)^{m+1}} \times \frac{1}{(1-t)^{m+1}} \\
&\times \frac{\pi N_{n_1 n_2 m}}{2\Gamma(1+i\beta)} \iiint \exp \left[ -p(\xi + \eta) - q(\xi - \eta) - u - \frac{a\xi s}{1-s} - \frac{a\eta t}{1-t} \right] \\
&\times (\xi\eta)^{m/2} u^{i\beta} \times J_m(\rho) J_m(\sigma) (\xi + \eta) du d\xi d\eta \\
&= \frac{1}{(1-s)^{m+1}} \times \frac{1}{(1-t)^{m+1}} \times \frac{\pi N_{n_1 n_2 m}}{2\Gamma(1+i\beta)} \frac{\partial U}{\partial p}, \quad (39)
\end{aligned}$$

where

$$\begin{aligned}
U &= \int u^{i\beta} e^{-u} du \times \int J_m(\rho) \xi^{m/2} \exp \left[ -(p+q) - \frac{as}{1-s} \right] \xi d\xi \\
&\times \int J_m(\sigma) \eta^{m/2} \exp \left[ -(p-q) - \frac{at}{1-t} \right] \eta d\eta. \quad (40)
\end{aligned}$$

The last two integrals are given by Watson<sup>25</sup> in the following form:

$$\int_0^\infty J_m(az) e^{-p^2 z^2} z^{m+1} dz = \frac{a^m}{(2p^2)^{m+1}} \exp \left[ -\frac{a^2}{4p^2} \right]. \quad (41)$$

Let  $z = \sqrt{\xi}$ . Introducing

$$P = (p+q) + \frac{as}{1-s}, \quad Q = (p-q) + \frac{at}{1-t}, \quad (42)$$

$$\rho_0^2 = -iku \sin^2\left(\frac{\theta_k}{2}\right), \quad \sigma_0^2 = -iku \cos^2\left(\frac{\theta_k}{2}\right), \quad (43)$$

we obtain

$$\left. \begin{aligned} \int J_m(\rho) \xi^{m/2} \exp\left\{-\left[p+q+\frac{\alpha s}{1-s}\right]\xi\right\} d\xi &= \frac{\rho_0^m \exp\left\{-\frac{\rho_0^2}{P}\right\}}{P^{m+1}}, \\ \int J_m(\sigma) \eta^{m/2} \exp\left\{-\left[p-q+\frac{\alpha t}{1-t}\right]\eta\right\} d\eta &= \frac{\sigma_0^m \exp\left\{-\frac{\sigma_0^2}{Q}\right\}}{Q^{m+1}}. \end{aligned} \right\} (44)$$

When equations (44) are substituted in equation (40),  $\rho_0$  and  $\sigma_0$  are eliminated through equations (43), and the integration is carried out with respect to  $u$ , we obtain

$$U = \left(\frac{-ik \sin \theta_k}{2}\right)^m \Gamma(m+1+i\beta) \times \frac{(PQ)^{i\beta}}{\left[PQ - ikQ \sin^2 \frac{\theta_k}{2} - ikP \cos^2 \frac{\theta_k}{2}\right]^{m+1+i\beta}}. \quad (45)$$

By definition of equations (42),

$$\begin{aligned} \frac{\partial U}{\partial p} &= \frac{\partial U}{\partial P} + \frac{\partial U}{\partial Q} = \left(\frac{-ik \sin \theta_k}{2}\right)^m \Gamma(i\beta+1+m) \\ &\times \frac{(PQ)^{i\beta-1}}{\left[PQ - ikQ \sin^2 \frac{\theta_k}{2} - ikP \cos^2 \frac{\theta_k}{2}\right]^{m+2+i\beta}} \\ &\times \left[\beta k \left(P^2 \cos^2 \frac{\theta_k}{2} + Q^2 \sin^2 \frac{\theta_k}{2}\right) - (m+1)PQ(P+Q-ik)\right]. \quad (46) \end{aligned}$$

Equation (39), with some modification in equation (46), can now be written

$$\begin{aligned}
\sum_{n_1 n_2} \frac{s^{n_1} t^{n_2} I(m n_1 n_2)}{(n_1 + m)! (n_2 + m)!} &= -\frac{\pi}{2} N_{n_1 n_2 m} \times \frac{(i\beta - m)!}{(i\beta)!} \times \left( \frac{-ik \sin \theta_k}{2} \right)^m \\
&\times [(1-s)(1-t)PQ]^{-(m+3)} \times \left[ 1 - ik \left( \frac{\sin^2 \frac{\theta_k}{2}}{P} + \frac{\cos^2 \frac{\theta_k}{2}}{Q} \right) \right]^{-(m+2+i\beta)} \\
&\times \left\{ (1-s)^2 (1-t)^2 \left[ \beta k \left( P^2 \cos^2 \frac{\theta_k}{2} + Q^2 \sin^2 \frac{\theta_k}{2} \right) - (m+1) PQ(P+Q-ik) \right] \right\}.
\end{aligned} \tag{47}$$

Expansion In Terms of s and t

Since  $I(m n_1 n_2)$  is independent of s and t, we can regard it as the coefficients of expansion of the right-hand side of equation (47) in powers of s and t. The expansion of the right-hand side is accomplished by a combination of the binomial and Taylor expansions.

Let us introduce a new complex variable a by

$$a = K - ia, \quad a^* = K + ia. \tag{48}$$

In terms of the new variable (cf., equations (38, 42)),

$$P = -\frac{i}{2} \times \frac{(a^* - k) - (a - k)s}{1 - s}, \quad Q = \frac{i}{2} \times \frac{(a + k) - (a^* + k)t}{1 - t}. \tag{49}$$

It follows that

$$\begin{aligned}
 [(1-s)P]^{-(m+3)} &= \left(-\frac{i}{2}\right)^{-(m+3)} [(a^* - k) - (a - k)s]^{-(m+3)} \\
 &= \left(-\frac{i}{2}\right)^{-(m+3)} \sum_{j_1=0}^{\infty} \binom{m+2+j_1}{j_1} (a^* - k)^{-(m+3+j_1)} (a - k)^{j_1} s^{j_1} ,
 \end{aligned} \tag{50}$$

$$\begin{aligned}
 [(1-t)Q]^{-(m+3)} &= \left(\frac{i}{2}\right)^{-(m+3)} [(a + k) - (a^* + k)t]^{-(m+3)} \\
 &= \left(\frac{i}{2}\right)^{-(m+3)} \sum_{j_2=0}^{\infty} \binom{m+2+j_2}{j_2} (a + k)^{-(m+3+j_2)} (a^* + k)^{j_2} t^{j_2} .
 \end{aligned} \tag{51}$$

Next, we introduce

$$\left. \begin{aligned}
 a_0 &= \frac{2 \sin^2 \frac{\theta_k}{2}}{a - k} , & a_1 &= \frac{a^* - k}{a - k} \\
 b_0 &= \frac{-2 \cos^2 \frac{\theta_k}{2}}{a^* + k} , & b_1 &= \frac{a + k}{a^* + k}
 \end{aligned} \right\} ; \tag{52}$$

then, if we set

$$y(s, t) = \left[ 1 - ik \left( \frac{\sin^2 \frac{\theta_k}{2}}{P} + \frac{\cos^2 \frac{\theta_k}{2}}{Q} \right) \right]^{-(m+2+i\beta)} , \tag{53}$$

through equations (49, 52) we can write

$$y(s, t) = \left[ 1 + k \left( a_0 \frac{1-s}{a_1-s} + b_0 \frac{1-t}{b_1-t} \right) \right]^{-(m+2+i\beta)} \equiv \sum_{\ell_1 \ell_2} \frac{y^{\ell_1 \ell_2}(0,0)}{\ell_1! \ell_2!} s^{\ell_1} t^{\ell_2}, \quad (54)$$

where on the right-hand side we have made a Taylor expansion,  $y^{\ell_1 \ell_2}(0,0)$  representing the  $\ell_1^{\text{th}}$  and the  $\ell_2^{\text{th}}$  derivatives of  $y(s, t)$  with respect to  $s$  and  $t$ , evaluated at  $s = t = 0$ . It is convenient to introduce two variables  $u$  and  $v$  given by

$$u = a_0 \frac{1-s}{a_1-s}, \quad v = b_0 \frac{1-t}{b_1-t}. \quad (55)$$

Then

$$y(u, v) = [1 + k(u + v)]^{-(m+2+i\beta)}. \quad (56)$$

It is also convenient to introduce

$$a_2 = a_0(1-a_1), \quad b_2 = b_0(1-b_1), \quad (57)$$

$$g = (a_1-s)^{-1}, \quad h = (b_1-t)^{-1}. \quad (58)$$

Then, making note of the relations

$$\frac{du}{ds} = a_2 g^2, \quad \frac{dv}{dt} = b_2 h^2,$$

$$\frac{d}{ds} g^n = n g^{n+1}, \quad \frac{d}{dt} h^n = n h^{n+1},$$

it follows that

$$y^{10}(s, t) = a_2 g^2 y'(u, v) ,$$

$$y^{20}(s, t) = a_2^2 g^4 y^2(u, v) + 2 a_2 g^3 y'(u, v) ,$$

$$y^{30}(s, t) = a_2^3 g^6 y^3(u, v) + 6 a_2^2 g^5 y^2(u, v) + 6 a_2 g^4 y'(u, v) ,$$

where  $y^\nu(u, v)$  is the  $\nu^{\text{th}}$  derivative of  $y(u, v)$  with respect to the arguments  $u$  or  $v$ . Inspection of the above equations shows that we can write in general

$$y^{\ell 0}(s, t) = \sum_{\nu=1}^{\ell} C(\nu, \ell) a_2^\nu g^{\ell+\nu} y^\nu(u, v) , \quad (59)$$

with  $C(\nu, \ell)$  some undetermined constants. The  $C(\nu, \ell)$  are found by differentiating equation (59) with respect to  $s$ :

$$\begin{aligned} y^{\ell+1,0}(s, t) &= \sum_{\nu=1}^{\ell+1} C(\nu, \ell+1) a_2^\nu g^{\ell+1+\nu} y^\nu \\ &= \sum_{\nu=1}^{\ell} \left[ (\ell+\nu) C(\nu, \ell) a_2^\nu g^{\ell+1+\nu} y^\nu \right. \\ &\quad \left. + C(\nu, \ell) a_2^{\nu+1} g^{\ell+2+\nu} y^{\nu+1} \right] . \end{aligned}$$

Comparison of the coefficients of  $a_2^\nu g^{\ell+1+\nu} y^\nu$  shows that

$$C(\nu, \ell + 1) = (\ell + \nu) C(\nu, \ell) + C(\nu - 1, \ell) . \quad (60)$$

Equation (60) gives the required recursion formula for  $C(\nu, \ell)$ . Inspection of the first few derivatives of  $y(s, t)$  shows that  $C(\nu, \ell) = 0$  when  $\nu = 0$  or  $\nu > \ell_1$ . This condition, the fact that  $C(1, 1) = 1$ , and equation (60) allow all the values of  $C(\nu, \ell)$  to be determined. The values of  $C(\nu, \ell)$  for the first few values of  $\ell$  are given in Table I.

Let us now write

$$y^{\ell_1 0}(s, t) = \sum_{\nu_1=1}^{\ell_1} C(\nu_1, \ell_1) a_2^{\nu_1} g^{\ell_1+\nu_1} y^{\nu_1}(u, v) .$$

By analogy we have similarly

$$y^{0 \ell_2}(s, t) = \sum_{\nu_2=1}^{\ell_2} C(\nu_2, \ell_2) b_2^{\nu_2} h^{\ell_2+\nu_2} y^{\nu_2}(u, v) .$$

For the combined derivative of  $y(s, t)$  we then obtain

$$\begin{aligned}
 y^{\ell_1 \ell_2}(s, t) &= \sum_{\nu_1=1}^{\ell_1} C(\nu_1, \ell_1) a_2^{\nu_1} g^{\ell_1+\nu_1} \frac{\partial^{\ell_2}}{\partial t^{\ell_2}} y^{\nu_1}(u, v) \\
 &= \sum_{\nu_1=1}^{\ell_1} C(\nu_1, \ell_1) a_2^{\nu_1} g^{\ell_1+\nu_1} \frac{\partial^{\nu_1}}{\partial u^{\nu_1}} \frac{\partial^{\ell_2}}{\partial t^{\ell_2}} y(u, v) \\
 &= \sum_{\nu_1=1}^{\ell_1} C(\nu_1, \ell_1) a_2^{\nu_1} g^{\ell_1+\nu_1} \frac{\partial^{\nu_1}}{\partial u^{\nu_1}} y^{0\ell_2}(s, t) \\
 &= \sum_{\nu_1=1}^{\ell_1} C(\nu_1, \ell_1) a_2^{\nu_1} g^{\ell_1+\nu_1} \times \sum_{\nu_2=1}^{\ell_2} C(\nu_2, \ell_2) b_2^{\nu_2} h^{\ell_2+\nu_2} y^{\nu_1+\nu_2}(u, v) .
 \end{aligned}$$

By introducing

$$C(0, 0) = 1 ,$$

and the fact that  $C(0, \ell) = 0$  for  $\ell \neq 0$ , the above equation may be written

$$y^{\ell_1 \ell_2}(s, t) = \sum_{\nu_1=0}^{\ell_1} \sum_{\nu_2=0}^{\ell_2} C(\nu_1, \ell_1) C(\nu_2, \ell_2) a_2^{\nu_1} b_2^{\nu_2} g^{\ell_1+\nu_1} h^{\ell_2+\nu_2} y^{\nu_1+\nu_2}(u, v) . \quad (61)$$

This equation is also valid when  $\ell_1 = \ell_2 = 0$ . By equation (56),

$$y^{\nu_1+\nu_2}(u, v) = \frac{(i\beta + m + 1 + \nu_1 + \nu_2)!}{(i\beta + m + 1)!} (-k)^{\nu_1+\nu_2} \times [1 + k(u + v)]^{-(i\beta + m + 2 + \nu_1 + \nu_2)} .$$

Through this equation and equations (55, 58) we obtain

$$\begin{aligned}
 y^{\ell_1 \ell_2} (0, 0) &= \sum_{\nu_1=0}^{\ell_1} \sum_{\nu_2=0}^{\ell_2} C(\nu_1, \ell_1) C(\nu_2, \ell_2) \times \frac{(i\beta + m + 1 + \nu_1 + \nu_2)!}{(i\beta + m + 1)!} (-k)^{\nu_1 + \nu_2} \\
 &\times a_2^{\nu_1} a_1^{-(\ell_1 + \nu_1)} b_2^{\nu_2} b_1^{-(\ell_2 + \nu_2)} \times \left[ 1 + k \left( \frac{a_0}{a_1} + \frac{b_0}{b_1} \right) \right]^{-(i\beta + m + 2 + \nu_1 + \nu_2)}
 \end{aligned}$$

The useful form of this equation is obtained when  $a_0, a_1, a_2, b_0, b_1, b_2$  are eliminated through equations (57, 52), and by putting  $\cos \theta_k = x$  (cf., equation (11)). The result is

$$\begin{aligned}
 y^{\ell_1 \ell_2} (0, 0) &= \sum_{\nu_1=0}^{\ell_1} \sum_{\nu_2=0}^{\ell_2} C(\nu_1, \ell_1) C(\nu_2, \ell_2) \times \frac{(i\beta + m + 1 + \nu_1 + \nu_2)!}{(i\beta + m + 1)!} \times (-k)^{\nu_1 + \nu_2} \\
 &\times (a - a^*)^{\nu_1 + \nu_2} \times [(a^* - k)(a + k)]^{i\beta + m + 2} \times (a - k)^{\ell_1 - \nu_1} \times (a^* - k)^{-(\ell_1 - \nu_2)} \\
 &\times (a + k)^{-(\ell_2 - \nu_1)} \times (a^* + k)^{\ell_2 - \nu_2} \times (1 - x)^{\nu_1} (1 + x)^{\nu_2} \\
 &\times [aa^* + k^2 - kx(a + a^*)]^{-(m + 2 + \nu_1 + \nu_2)}. \quad (62)
 \end{aligned}$$

This completes the expansion of equation (53).

Finally, for the last  $s, t$  dependent term in equation (47), through equation (49) it follows that

$$\begin{aligned}
& (1-s)^2 (1-t)^2 \left[ \beta k \left( P^2 \cos^2 \frac{\theta_k}{2} + Q^2 \sin^2 \frac{\theta_k}{2} \right) - (m+1) PQ(P+Q-ik) \right] \\
&= -\frac{1}{4} \beta k \cos^2 \frac{\theta_k}{2} [(a^*-k) - (a-k)s]^2 (1-t)^2 \\
&\quad - \frac{1}{4} \beta k \sin^2 \frac{\theta_k}{2} [(a+k) - (a^*+k)t]^2 (1-s)^2 \\
&\quad - \frac{1}{4} \alpha(m+1) [(a^*-k) - (a-k)s] [(a+k) - (a^*+k)t] (1-st) \\
&\equiv \sum_{\mu_1=0}^2 \sum_{\mu_2=0}^2 A_{\mu_1 \mu_2} s^{\mu_1} t^{\mu_2} \quad , \quad (63)
\end{aligned}$$

where it is desirable to find the coefficients  $A_{\mu_1 \mu_2}$ . To accomplish this, we introduce two angles  $\phi_1$  and  $\phi_2$  such that

$$\phi_1 = \tan^{-1} \frac{\alpha}{k-K} \quad , \quad \phi_2 = \tan^{-1} \frac{\alpha}{k+K} \quad , \quad 0 < \phi_1, \phi_2 < \pi \quad . \quad (64)$$

In this way we get

$$\begin{aligned}
\sum_{\mu_1 \mu_2} A_{\mu_1 \mu_2} s^{\mu_1} t^{\mu_2} &= -\frac{1}{4} \beta k \cos^2 \frac{\theta_k}{2} (a^* - k)^2 \left[1 - e^{2i\phi_1} s\right]^2 (1-t)^2 \\
&\quad - \frac{1}{4} \beta k \sin^2 \frac{\theta_k}{2} (a+k)^2 \left[1 - e^{2i\phi_2} t\right]^2 (1-s)^2 \\
&\quad - \frac{1}{4} \alpha(m+1) (a^* - k) (a+k) \left[1 - e^{2i\phi_1} s\right] \left[1 - e^{2i\phi_2} t\right] (1-st) \\
&= -\frac{1}{4} \beta k \cos^2 \frac{\theta_k}{2} (a^* - k)^2 \sum_{\mu_1=0}^2 \sum_{\mu_2=0}^2 (-)^{\mu_1 + \mu_2} \binom{2}{\mu_1} \binom{2}{\mu_2} e^{2i\mu_1 \phi_1} s^{\mu_1} t^{\mu_2} \\
&\quad - \frac{1}{4} \beta k \sin^2 \frac{\theta_k}{2} (a+k)^2 \sum_{\mu_1=0}^2 \sum_{\mu_2=0}^2 (-)^{\mu_1 + \mu_2} \binom{2}{\mu_1} \binom{2}{\mu_2} e^{2i\mu_2 \phi_2} s^{\mu_1} t^{\mu_2} \\
&\quad - \frac{1}{4} \alpha(m+1) (a^* - k) (a+k) \left[ \sum_{\mu_1=0}^2 \sum_{\mu_2=0}^2 [1 - \delta(\mu_1, 2)] [1 - \delta(\mu_2, 2)] (-)^{\mu_1 + \mu_2} \right. \\
&\quad \times e^{2i(\mu_1 \phi_1 + \mu_2 \phi_2)} s^{\mu_1} t^{\mu_2} - \sum_{\mu_1=0}^2 \sum_{\mu_2=0}^2 [1 - \delta(\mu_1, 0)] [1 - \delta(\mu_2, 0)] (-)^{\mu_1 + \mu_2} \\
&\quad \left. \times e^{2i[(\mu_1 - 1)\phi_1 + (\mu_2 - 1)\phi_2]} s^{\mu_1} t^{\mu_2} \right].
\end{aligned}$$

By equating the coefficients of  $s^{\mu_1} t^{\mu_2}$ , we obtain

$$\begin{aligned}
A_{\mu_1 \mu_2} &= -\frac{1}{4} \beta k (-)^{\mu_1 + \mu_2} \binom{2}{\mu_1} \binom{2}{\mu_2} \left[ (a^* - k)^2 e^{2i\mu_1 \phi_1} \cos^2 \frac{\theta_k}{2} + (a + k)^2 e^{2i\mu_2 \phi_2} \sin^2 \frac{\theta_k}{2} \right] \\
&\quad - \frac{1}{4} \alpha(m+1) (-)^{\mu_1 + \mu_2} (a^* - k)(a + k) \left[ \bar{\delta}(\mu_1, \mu_2, 22) e^{2i(\mu_1 \phi_1 + \mu_2 \phi_2)} \right. \\
&\quad \left. - \bar{\delta}(\mu_1, \mu_2, 00) e^{2i[(\mu_1 - 1)\phi_1 + (\mu_2 - 1)\phi_2]} \right], \tag{65}
\end{aligned}$$

where we have defined

$$\bar{\delta}(\mu_1, \mu_2, n_1, n_2) = \left[ 1 - \delta(\mu_1, n_1) \right] \times \left[ 1 - \delta(\mu_2, n_2) \right]. \tag{66}$$

When  $x = \cos \theta_k$  is introduced and we set

$$A_{\mu_1 \mu_2} = B_{\mu_1 \mu_2} + x C_{\mu_1 \mu_2}, \tag{67}$$

we obtain, since  $\beta k = Z$ ,

$$\begin{aligned}
B_{\mu_1 \mu_2} &= -\frac{Z}{8} (-)^{\mu_1 + \mu_2} \binom{2}{\mu_1} \binom{2}{\mu_2} \left[ (a^* - k)^2 e^{2i\mu_1 \phi_1} + (a + k)^2 e^{2i\mu_2 \phi_2} \right] \\
&\quad - \frac{\alpha}{4} (m+1) (-)^{\mu_1 + \mu_2} (a^* - k)(a + k) \left[ \bar{\delta}(\mu_1, \mu_2, 22) - \bar{\delta}(\mu_1, \mu_2, 00) e^{-2i(\phi_1 + \phi_2)} \right] e^{2i(\mu_1 \phi_1 + \mu_2 \phi_2)}, \tag{68}
\end{aligned}$$

$$C_{\mu_1 \mu_2} = -\frac{Z}{8} (-)^{\mu_1 + \mu_2} \binom{2}{\mu_1} \binom{2}{\mu_2} \left[ (a^* - k)^2 e^{2i\mu_1 \phi_1} - (a + k)^2 e^{2i\mu_2 \phi_2} \right]. \tag{69}$$

Returning to equation (47) and referring to equations (50, 51, 53, 54, 63), we can write finally

$$\begin{aligned}
\sum_{n_1 n_2} \frac{s^{n_1} t^{n_2} I(mn_1 n_2)}{(n_1 + m)!(n_2 + m)!} &= -\frac{\pi}{2} (4)^{m+3} N_{n_1 n_2 m} \times \frac{(i\beta + m)!}{(i\beta)!} \times \left(\frac{-ik}{2}\right)^m (1-x^2)^{m/2} \\
&\times \sum_{j_1=0}^{\infty} \sum_{j_2=0}^{\infty} \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} \sum_{\mu_1=0}^2 \sum_{\mu_2=0}^2 \binom{m+2+j_1}{j_1} \binom{m+2+j_2}{j_2} (a^* - k)^{-(m+3+j)} \times (a - k)^{j_1} \\
&\times (a + k)^{-(m+3+j_2)} \times (a^* + k)^{j_2} \times [\ell_1! \ell_2!]^{-1} y^{\ell_1 \ell_2} (0, 0) A_{\mu_1 \mu_2} \times s^{j_1 + \ell_1 + \mu_1} \times t^{j_2 + \ell_2 + \mu_2}.
\end{aligned} \tag{70}$$

$I(mn_1 n_2)$  is found by equating coefficients of equal powers of  $s$  and  $t$  on both sides of this equation, and substituting the values of  $y^{\ell_1 \ell_2} (0, 0)$  and  $A_{\mu_1 \mu_2}$  from equations (62, 67):

$$\begin{aligned}
I(mn_1 n_2) &= -\frac{\pi}{2} (4)^{m+3} (n_1 + m)!(n_2 + m)! N_{n_1 n_2 m} \frac{(i\beta + m)!}{(i\beta)!} \times \left(\frac{-ik}{2}\right)^m (1-x^2)^{m/2} \\
&\times [(a^* - k)(a + k)]^{i\beta-1} \sum_{\substack{j_1 \ell_1 \mu_1 \\ j_2 \ell_2 \mu_2}} [\ell_1! \ell_2!]^{-1} \binom{m+2+j_1}{j_1} \binom{m+2+j_2}{j_2} \\
&\times \left(\frac{a-k}{a^*-k}\right)^{j_1 + \ell_1} \times \left(\frac{a^*+k}{a+k}\right)^{j_2 + \ell_2} \times [B(\mu_1 \mu_2) + xC(\mu_1 \mu_2)] \\
&\times \sum_{\nu_1=0}^{\ell_1} \sum_{\nu_2=0}^{\ell_2} C(\nu_1, \ell_1) C(\nu_2, \ell_2) \times \frac{(i\beta + m + 1 + \nu_1 + \nu_2)!}{(i\beta + m + 1)!} \times (k)^{\nu_1 + \nu_2} \times (2i\alpha)^{\nu_1 + \nu_2} \\
&\times \left(\frac{a+k}{a-k}\right)^{\nu_1} \times \left(\frac{a^*-k}{a^*+k}\right)^{\nu_2} (1-x)^{\nu_1} (1+x)^{\nu_2} \times [aa^* + k^2 - kx(a + a^*)]^{-(m+2+\nu_1+\nu_2)},
\end{aligned} \tag{71}$$

where the summation over  $j_1 \ell_1 \mu_1$ , and  $j_2 \ell_2 \mu_2$  is subject to the conditions

$$\left. \begin{aligned} j_1 + \ell_1 + \mu_1 &= n_1, \\ j_2 + \ell_2 + \mu_2 &= n_2. \end{aligned} \right\} \quad (72)$$

Let us designate the set of integers  $j_1 \ell_1 \nu_1 \mu_1 j_2 \ell_2 \nu_2 \mu_2$  by  $\gamma$ ,

$$\gamma = (j_1 \ell_1 \nu_1 \mu_1 j_2 \ell_2 \nu_2 \mu_2), \quad (73)$$

and introduce the angle  $\phi_3$  through

$$\phi_3 = \tan^{-1} \frac{2ak}{K^2 + a^2 - k^2}, \quad 0 \leq \phi_3 < \pi. \quad (74)$$

Taking note of  $\beta = Z/k$  and equations (48, 64), the  $I(mn_1 n_2)$  — neglecting an arbitrary phase factor — reduces to

$$\begin{aligned} I(mn_1 n_2) &= (2)^{m+5} \pi (n_1 + m)! (n_2 + m)! N_{n_1 n_2 m} (iZ + (m+1)k)^{-1} \\ &\times \left[ (K^2 + a^2 + k^2)^2 - 4k^2 K^2 \right]^{-1/2} e^{-\beta \phi_3} \sum_{\gamma} G(\gamma) H(\gamma), \quad (75) \end{aligned}$$

$$\begin{aligned} G(\gamma) &= \binom{m+2+j_1}{j_1} \binom{m+2+j_2}{j_2} (\ell_1! \ell_2!)^{-1} C(\nu_1, \ell_1) C(\nu_2, \ell_2) (2i\alpha)^{\nu_1 + \nu_2} \\ &\left[ \prod_{\omega=1}^{m+1+\nu_1+\nu_2} (iZ + \omega k) \right] \left( \frac{a+k}{a-k} \right)^{\nu_1} \times \left( \frac{a^* - k}{a^* + k} \right)^{\nu_2} \exp 2i \left[ (j_1 + \ell_1) \phi_1 + (j_2 + \ell_2) \phi_2 \right], \quad (76) \end{aligned}$$

$$\begin{aligned}
H(\gamma) &= (1-x^2)^{m/2} (1-x)^{\nu_1} (1+x)^{\nu_2} \left[ B(\mu_1, \mu_2) + xC(\mu_1, \mu_2) \right] \\
&\times \left[ aa^* + k^2 - kx(a + a^*) \right]^{-(m+2+\nu_1+\nu_2)} .
\end{aligned} \tag{77}$$

Substitution of equation (75) in equation (36) and elimination of  $N_{n_1 n_2 m}$  through equation (20) give

$$\begin{aligned}
Q_{(nmn_1 n_2)} &= \frac{\pi 2^8 (2\alpha)^{2m+4}}{k_0^2} \times \frac{n_1! n_2!}{(n_1+m)! (n_2+m)!} \int_{k=0}^{k_{\max}} \frac{k dk}{[Z^2 + (m+1)^2 k^2] [1 - e^{-\pi Z/k}]} \\
&\times \int_{k_0-k_1}^{k_0+k_1} \frac{e^{-2Z\phi_3/k} dK}{K^3 [(\alpha^2 + K^2 + k^2)^2 - 4k^2 K^2]} \times S(k, K) ,
\end{aligned} \tag{78}$$

where

$$\begin{aligned}
S(k, K) &= \int_{-1}^{+1} \left| \sum_{\gamma} G(\gamma) H(\gamma) \right|^2 dx \\
&= \sum_{\gamma} \sum_{\gamma'} G(\gamma) G^*(\gamma') \int_{-1}^{+1} H(\gamma) H^*(\gamma') dx .
\end{aligned} \tag{79}$$

The integration over  $x$  can be carried out by ordinary methods. Let us call the integral with respect to  $x$ ,  $\mathfrak{A}(\gamma\gamma')$ ; then, through binomial

expansions,

$$\begin{aligned}
\mathcal{J}(\gamma\gamma') &= \int_{-1}^{+1} H(\gamma) H^*(\gamma') dx = \int_{-1}^{+1} (1-x^2)^m (1-x)^{\nu_1+\nu_1'} (1+x)^{\nu_2+\nu_2'} \\
&\times [B(\mu_1 \mu_2) + xC(\mu_1 \mu_2)] [B^*(\mu_1' \mu_2') + xC^*(\mu_1' \mu_2')] (A+Bx)^{-g} dx \\
&= \sum_{m_1=0}^m (-)^{m_1} \binom{m}{m_1} \sum_{t=0}^1 \sum_{t'=0}^1 B(\mu_1 \mu_2)^{1-t} C(\mu_1 \mu_2)^t B^*(\mu_1' \mu_2')^{1-t'} C^*(\mu_1' \mu_2')^{t'} \\
&\times \sum_{h_1=0}^{\nu_1+\nu_1'} \sum_{h_2=0}^{\nu_2+\nu_2'} (-)^{h_1} \binom{\nu_1+\nu_1'}{h_1} \binom{\nu_2+\nu_2'}{h_2} \int_{-1}^{+1} x^M (A+Bx)^{-g} dx, \quad (80)
\end{aligned}$$

where we have expressed

$$\left. \begin{aligned}
A &= aa^* + k^2 = K^2 + a^2 + k^2, & B &= -k(a+a^*) = -2kK, \\
g &= 2(m+2) + \nu_1 + \nu_2 + \nu_1' + \nu_2', & M &= 2m_1 + t + t' + h_1 + h_2.
\end{aligned} \right\} (81)$$

The integral with respect to  $x$  in equation (80) is evaluated in Appendix I and is designated by  $J(M, g)$ . For future reference the key equations in ionization are listed below.

### Summary of the Equations

Suppose the initial state of the atom with a nucleus of charge  $Z$  be specified by  $nm_1 n_2$ , the magnitude of the momentum of the ionizing electron before collision by  $k_0$ , the magnitude of the momentum transfer

by  $K$ , and the magnitude of the momentum of the ejected electron by  $k$ ; the total ionization cross section is then given by

$$Q(nm n_1 n_2) = 2 \int_{k=0}^{k_{\max}} q(nm n_1 n_2 | k) k dk, \quad (S1)$$

$$q(nm n_1 n_2 | k) = \frac{\pi 2^7 (2\alpha)^{2m+4}}{k_0^2} \times \frac{n_1! n_2!}{(n_1+m)! (n_2+m)!} \times \frac{1}{[Z^2 + (m+1)^2 k^2] [1 - e^{-2\pi Z/k}]} \\ \times \int_{k_0-k_1}^{k_0+k_1} \frac{e^{-2Z\phi_3/k} dK}{K^3 [(\alpha^2 + K^2 + k^2)^2 - 4k^2 K^2]} \times S(k, K), \quad (S2)$$

where

$$S(k, K) = \sum_{\gamma} \sum_{\gamma'} G(\gamma) G^*(\gamma') \mathfrak{L}(\gamma, \gamma'). \quad (S3)$$

In this equation  $\gamma$  stands for 8 integers,

$$\gamma = (j_1 \ell_1 \nu_1 \mu_1 j_2 \ell_2 \nu_2 \mu_2), \quad (S4)$$

which combine according to

$$\left. \begin{aligned} j_1 + \ell_1 + \mu_1 &= n_1; & j_1, \ell_1 &= 0, 1, 2, 3, \dots \\ \mu_1 &= 0, 1, 2; & \nu_1 &= 0, 1, 2, \dots, \ell_1; \\ j_2 + \ell_2 + \mu_2 &= n_2; & j_2, \ell_2 &= 0, 1, 2, 3, \dots \\ \mu_2 &= 0, 1, 2; & \nu_2 &= 0, 1, 2, \dots, \ell_2. \end{aligned} \right\} \quad (S5)$$

The explicit forms of  $G(\gamma)$  and  $\mathfrak{L}(\gamma, \gamma')$  are

$$G(\gamma) = \binom{m+2+j_1}{j_1} \binom{m+2+j_2}{j_2} (\ell_1! \ell_2!)^{-1} C(\nu_1 \ell_1) C(\nu_2 \ell_2) (2ia)^{\nu_1+\nu_2} \\ \times \left[ \prod_{\omega=1}^{m+1+\nu_1+\nu_2} (iZ + \omega k) \right] \left( \frac{a+k}{a-k} \right)^{\nu_1} \left( \frac{a^*-k}{a^*+k} \right)^{\nu_2} \exp 2i [(j_1 + \ell_1) \phi_1 + (j_2 + \ell_2) \phi_2], \quad (S6)$$

$$\mathfrak{L}(\gamma\gamma') = \sum_{m_1=0}^m (-)^{m_1} \binom{m}{m_1} \sum_{t=0}^1 \sum_{t'=0}^1 B_{\mu_1\mu_2}^{1-t} C_{\mu_1\mu_2}^t B_{\mu_1\mu_2}^{*1-t'} C_{\mu_1\mu_2}^{*t'} \\ \times \sum_{h_1=0}^{\nu_1+\nu_1'} \sum_{h_2=0}^{\nu_2+\nu_2'} (-)^{h_1} \binom{\nu_1+\nu_1'}{h_1} \binom{\nu_2+\nu_2'}{h_2} J(M, g) \quad , \quad (S7)$$

$J(M, g)$  being given in Appendix I.

The parameters  $a, \phi_1, \phi_2, \phi_3, \alpha, C(\nu, \ell), B_{\mu_1\mu_2}$ , and  $C_{\mu_1\mu_2}$  are defined in the text.

We recognize  $q(nm n_1 n_2 | k)$  as the ionization cross section per unit rydberg energy of the ejected electron.

### Symmetry Considerations

Equation (31) shows that, when  $\zeta, \eta; K, -K; n_1, n_2$ ; and  $\sin \frac{\theta_k}{2}, \cos \frac{\theta_k}{2}$  are interchanged,  $V(\mathbf{k}, K)$  remains invariant. Since  $\zeta$  and  $\eta$  are the variables of integrations, the interchange of  $\zeta$  and  $\eta$  does not change  $V(\mathbf{k}, K)$  in any case. By putting  $\cos \theta_k = x$ , this means that  $V(\mathbf{k}, K)$  does not change under the following interchanges

$$K \rightleftharpoons -K, \quad n_1 \rightleftharpoons n_2, \quad x \rightleftharpoons -x.$$

We consider the integral

$$\int_{-1}^{+1} |V(k, K, n)|^2 dx ,$$

which is the form that appears in the expression for the cross section. The integrand can be written as the sum of odd and even functions of  $x$ . The integral with respect to the odd function is zero. The integral with respect to the even function does not change when  $x \rightarrow -x$ . Then the above integral is invariant under the interchanges  $K \rightarrow -K$ ,  $n_1 \rightarrow n_2$ . Or, by equation (10), the interchange of the quantum numbers  $n_1$  and  $n_2$  is equivalent to the change of sign of  $K$  in the expression for the integrand with respect to  $k$  and  $K$  of the cross section. Formally, through equation (78) this can be written

$$S(n_2 n_1 | kK) = S(n_1 n_2 | k - K) .$$

A further symmetry exists with respect to  $k$ . By equation (35),

$$I(mn_1 n_2 | -k - K\theta_k) = I^*(mn_1 n_2 | kK\theta_k) .$$

Through equations (75, 79) it also is true that

$$S(n_1 n_2 | -k - K) = S(n_1 n_2 | kK) .$$

Combining with the previous result, it follows that

$$S(n_2 n_1 | k, K) = S(n_1 n_2 | k, -K) = S(n_1 n_2 | -k, K) . \quad (82)$$

A case of particular interest is the ionization with zero momentum ejected electron,  $k = 0$ ; this corresponds to the excitation of the hydrogen atom to the state  $n \rightarrow \infty$ . Equation (S2) shows that this cross section does not change with the interchange of  $n_1$  and  $n_2$  :

$$q(nm n_2 n_1 | 0) = q(nm n_1 n_2 | 0) . \quad (83)$$

### Multiplicity of States and the Total Cross Section

Since  $n_1 + n_2 = n - m - 1$ ,  $n_1$  can take the values  $0, 1, 2, \dots, n - m - 1$ ; or  $n - m$  values. The same is true of  $n_2$ . Then the total number of combinations of  $n_1$  and  $n_2$  for a given  $n$  and  $m$  is  $n - m$ . The average value of cross section for a given  $n$  and  $m$  is therefore

$$Q(nm) = (n - m)^{-1} \sum_{n_1 n_2} Q(nm n_1 n_2) . \quad (84)$$

For a given  $n$  the total number of states with different  $m$  is  $2n - 1$ . The average cross section for a given  $n$  is therefore

$$Q(n) = (2n - 1)^{-1} \sum_{m=0}^{n-1} \epsilon_m Q(nm) , \quad (85)$$

$\epsilon_m$  defined in equation (21). Notice that the total number of states for a given  $n$  is

$$N = \sum_{m=0}^{n-1} [2 - \delta(m, 0)] (n - m) = n + 2 \left[ n(n - 1) - \frac{n}{2} (n - 1) \right] = n^2 ,$$

as it should be.

### III. RESULTS AND DISCUSSION

We have calculated, using Eqs. (78, 79), the ionization of all sublevels of hydrogen belonging to the principal quantum numbers  $n = 1, 2, 3, 4, 5$ . We also have computed the ionization of one sublevel for each of the principal quantum numbers  $n = 6, 7, 8, 9, 10$ . Since the ionization cross section of all sublevels of any principal quantum number is approximately the same in parabolic coordinates, the latter calculation gives an indication of the ionization cross section of  $n = 6, 7, 8, 9, 10$ . Thus we have at our disposal the ionization cross section of the first 10 levels of the hydrogen.

To test the accuracy of our results we have compared them with those of the spherical coordinates. For the ground state, the wave function in the two coordinates is the same. Table I compares the results in the two coordinates. The ionization cross section in spherical coordinates was first calculated by Massey and Mohr<sup>2</sup>. Here it has been recalculated. The agreement between the results of the two coordinates is excellent.

The results of  $n = 2$  levels, again in both coordinates, are given in Table II. For  $m = 1$  the wave function in both coordinates is the same. The agreement is shown in this table and Fig. 1. For  $m = 0$  the wave function of hydrogen in parabolic coordinates is related to the wave function in spherical coordinates through

$$\begin{aligned}
\phi(20\ 10) &= \frac{1}{\sqrt{2}} [\phi(2s) + \phi(2p0)] \\
\phi(20\ 01) &= \frac{1}{\sqrt{2}} [\phi(2s) - \phi(2p0)] .
\end{aligned}
\left. \vphantom{\begin{aligned} \phi(20\ 10) \\ \phi(20\ 01) \end{aligned}} \right\} \quad (86)$$

These are incidently the wave functions used in the first order Stark effect. Substitution of these as the initial wave functions in Eqs. (8, 10) shows that we must have

$$Q(20\ 10) + Q(20\ 01) = Q(2s) + Q(2p0) , \quad (87)$$

$Q(nm\ n_1\ n_2)$  being the ionization cross section of the state specified by  $n\ m\ n_1\ n_2$ . Table II shows that the above equation is numerically satisfied; this is further shown in Fig. 2.

Originally the ionization of the 2s and the  $2p, m = 0$  states was formulated by Burhop<sup>3</sup> and computed numerically by Swan<sup>6</sup>. Swan's results are larger approximately by a factor of 2 due to being unduly multiplied by a factor of 2 and being obtained by a cruder method of numerical integration. Boyd<sup>26</sup>, and McCrea and McKirgan<sup>27</sup> in determination of the ionization with zero velocity ejected electrons of the 2s and the  $2p, m = 0$  states find similar discrepancies.

At the moment, aside from the Born approximation, the most important calculation of ionization with applicability to higher states is the classical calculation. J. J. Thomson<sup>1</sup> in 1912, following his model of atoms with stationary electrons, considered the collision of a moving

electron with an electron at rest caused by their mutual coulomb interaction. When the energy imparted to the electron at rest exceeds its bound energy, the ionization takes place. Since the imparted energy decreases as the impact parameter increases, an integration with respect to the impact parameter between zero and a fixed limit gives the ionization cross section. The result is

$$Q_i = \frac{4}{E_0} \left( n^2 - \frac{1}{E_0} \right), \quad (88)$$

where  $Q_i$  is the cross section in units of  $\pi a_0^2$ ,  $E_0$  the impact energy in rydberg, and  $n$  is the principal quantum number of the atom. The result of this simple classical calculation is in fair agreement with experiment and the elaborate quantum mechanical Born calculation, although it gives a smaller cross section and the position of the maximum cross section is displaced. A major improvement in Thomson's calculation is to take the motion of the bound electron into account. This has been done by Gryzinski<sup>28</sup>. Let us introduce  $a = (n^2 E_0)^{-1}$ , then according to Gryzinski Eq. (88) should be replaced by

$$Q_i = \sigma_0 n^4 g(n, E_0), \quad (89)$$

where  $\sigma_0 = 4.0307 \pi a_0^2$  and

$$g(n, E_0) = a(1+a)^{-3/2} \times \begin{cases} \left( \frac{5}{3} - 2a \right), & a \leq \frac{1}{2} \\ \frac{4\sqrt{2}}{3} (1-a)^{3/2}, & a \geq \frac{1}{2} \end{cases} \quad (90)$$

It should be noticed that in both Eqs. (88, 89) the cross section falls off asymptotically as  $E_0^{-1}$  while in quantum mechanical Born calculation the corresponding asymptotic form is  $\log E_0/E_0$ <sup>29</sup>.

For comparison, in Fig. 3 the Born, classical and experimental curves are drawn. It is seen that close to the threshold the experimental curve agrees better with the classical but asymptotically it favors the quantum mechanical calculations.

The ionization of the  $n = 3, 4, 5$  levels are given in Tables III, IV and V. Table VI gives the ionization of the sublevel with the greatest magnetic quantum number for each of the levels  $n = 6, 7, 8, 9,$  and 10. Fig. 4 corresponds to the ionization of the  $n = 2$  while Fig. 5 gives the ionization cross sections of all sublevels of the  $n = 3$ . Figs. 6, 7, 8 give the ionization curves for the levels  $n = 3, 4, 5$ . The cross section for each level is in units of  $n^4 \pi a_0^2$ , which is the geometrical cross section of the level concerned. Along each level ionization curve the classical curve is also drawn for comparison. Fig. 9 gives the ionization of one component of each of the levels  $n = 6, 7, 8, 9, 10$ . It is interesting to note that with increasing  $n$ , the cross section does not increase as rapidly as the fourth power of  $n$ .

Table VII gives the partial ionization cross section, i.e., ionization cross section per unit rydberg energy of the ejected electron, for the five levels  $n = 1, 2, 3, 4, 5$ . Finally Figs. 10-14 give the corresponding curves for these cross sections. The maxima of the partial cross sections occur when the velocity of the ejected electron is half its velocity before ejection. The reason for this is not understood yet.

With regard to numerical integration, when the number of values of  $\gamma$  given by Eq. (73) is small, the closed form has been used while the integral form has been more convenient when the number of values of  $\gamma$  is large.

## ACKNOWLEDGMENT

The solution to this problem was initiated through a discussion with Dr. M. Lecar of the Goddard Institute for Space Studies and Yale University, who needed the ensuing results in his astrophysical calculations. The programming was done by E. Sullivan, whom I wish to thank for his keen interest in this complex problem. I wish also to thank the Computing Branch of the Theoretical Division for providing their generous services.

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## APPENDIX I

### Integration with Respect to x

Let us set

$$J(M, g) = \int_{-1}^{+1} x^M (A + Bx)^{-g} dx ,$$

$$M = 2m_1 + t + t' + h_1 + h_2 , \quad g = 2(m+2) + \nu_1 + \nu_2 + \nu_1' + \nu_2' ,$$

$$A = K^2 + \alpha^2 + k^2 , \quad B = -2kK .$$

Introducing  $X = A + Bx$ , we obtain

$$\begin{aligned} J(M, g) &= B^{-(M+1)} \int_{A-B}^{A+B} (X-A)^M X^{-g} dX = B^{-(M+1)} \sum_{s=0}^M \binom{M}{s} (-A)^s \int_{A-B}^{A+B} X^{M-s-g} dX \\ &= B^{-(M+1)} \sum_{s=0}^M \binom{M}{s} (-A)^s \times \begin{cases} \frac{1}{N} [(A+B)^N - (A-B)^N] , & N \neq 0 \\ \ln \frac{A+B}{A-B} , & N = 0 , \end{cases} \end{aligned}$$

$$N = M - s - g + 1 . \quad (A1)$$

When  $k \neq 0$ , an alternative form can be found. Noticing that

$$(A + Bx)^{-g} = A^{-g} \left(1 + \frac{Bx}{A}\right)^{-g} = A^{-g} \sum_{s=0}^{\infty} \binom{g-1+s}{s} \left(-\frac{Bx}{A}\right)^s ,$$

we get

$$J(M, g) = A^{-g} \sum_{s=0}^{\infty} \frac{1 - (-1)^{M+s+1}}{M+s+1} \binom{g-1+s}{s} \left(\frac{-B}{A}\right)^s \quad (A2)$$

TABLE I

The  $C(\nu, l)$  values.

$\nu \backslash l$	0	1	2	3	4	5
0	1	0	0	0	0	0
1	0	1	0	0	0	0
2	0	2	1	0	0	0
3	0	6	6	1	0	0
4	0	24	36	12	1	0
5	0	120	240	120	20	1

Table I. Cross sections in units of  $\pi a_0^2$  for the ionization of the hydrogen atom in  $n = 1$  level by electron collision, calculated in the Born approximation.  $Q(1s)$  is the calculated cross section employing the spherical coordinates while  $Q(1000)$  is the same cross section employing the parabolic coordinate.

Impact Energy		Q(1000)	Q(1s)
ryd	eV		
1.00	13.6	0.0	0.0
1.44	19.6	0.57555	0.57502
1.96	26.7	1.0016	0.99797
2.00	27.2	1.0168	
2.56	34.8	1.1691	1.1691
3.24	44.1	1.1931	1.1931
4.00	54.4	1.1449	1.1449
6.25	85.0	0.93696	0.93660
9.00	122.4	0.74243	0.74244
12.25	166.6	0.59375	0.59367
16.00	217.6	0.48282	0.48283
20.25	275.4	0.39959	0.39959

Table II. Cross sections in units of  $\pi a_0^2$  for the ionization of the hydrogen atom in  $n = 2$  level by electron collision, calculated in the Born approximation.  $Q(2s)$ ,  $Q(2p, m=0)$  and  $Q(2p, m = 1)$ , with  $m$  the absolute value of the magnetic quantum number, are the calculated cross sections for the sublevels of  $n = 2$  in spherical coordinates.  $Q(n m n_1 n_2)$  are the calculated cross sections for the sublevels of  $n = 2$  in parabolic coordinates.  $\bar{Q}(2)$  is the averaged cross section for  $n = 2$  level.

Impact Energy		$Q(2p, m=1)$	$Q(2100)$	$Q(2s)$	$Q(2p, m=0)$	$Q(2s) + Q(2p, m=0)$	$Q(2010)$	$Q(2001)$	$Q(2010) + Q(2001)$	$\bar{Q}(2)$
ryd	eV									
0.25	3.4	0	0	0	0	0	0	0	0	0
0.36	4.9	10.80	10.86	10.77	9.387	20.16	10.14	10.14	20.28	10.50
0.50	6.8		17.485				17.142	17.139		17.312
0.64	8.7	19.11	19.11	17.62	20.96	38.58	19.29	19.29	38.58	19.20
1.00	13.6	17.37	17.37	16.04	20.58	36.62	18.31	18.31	36.62	17.84
1.44	19.6	14.14	14.20	13.31	17.34	30.65	15.35	15.35	30.70	14.78
3.24	44.1	7.584	7.584	7.549	9.599	17.148	8.575	8.574	17.149	8.079
5.29	71.9	4.956	4.956	5.079	6.326	11.405	5.703	5.702	11.405	5.329
7.29	99.1	3.721	3.722	3.877	4.766	8.643	4.322	4.322	8.644	4.022

Table III. Cross sections in units of  $\pi a_0^2$  for the ionization of the hydrogen atom in  $n = 3$  level by electron collision, calculated in the Born approximation and employing the parabolic coordinates. The cross section of each sublevel is designated by  $Q(n m n_1 n_2)$ . Three of the six sublevels with their  $m \neq 0$  are doubly degenerate, hence the six sublevels constitute the nine components of  $n = 3$ .  $\bar{Q}(3)$  is the averaged cross section for  $n = 3$  level.

Impact Energy		Q(3200)	Q(3110)	Q(3101)	Q(3020)	Q(3002)	Q(3011)	$\bar{Q}(3)$
ryd	eV							
0.11	1.5	0	0	0	0	0	0	0
0.16	2.2	60.054	56.175	56.183	50.836	51.055	56.920	55.960
0.22	3.0	91.54	92.99	92.78	89.40	88.95	93.60	91.84
0.36	4.9	91.259	99.532	99.326	101.27	100.80	99.542	97.98
0.64	8.7	66.031	75.403	75.237	80.148	79.958	75.239	74.298
1.0	13.6	46.370	54.149	54.082	55.867	59.127	49.338	52.615
4.0	54.4	13.262	15.847	15.793	17.528	14.072	13.633	15.004

Table IV. Cross sections in units of  $\pi a_0^2$  for the ionization of the hydrogen atom in  $n = 4$  level by electron collision, calculated in the Born approximation and employing the parabolic coordinates. The cross section of each sublevel is designated by  $Q(n m n_1 n_2)$ . With the six of the sublevel cross sections listed doubly degenerate, the list of the 16 components of  $n = 4$  level is complete.  $\bar{Q}(4)$  is the averaged cross section for  $n = 4$  level.

Energy Impact ryd	Energy Impact eV														
	Q(4300)	Q(4210)	Q(4201)	Q(4120)	Q(4102)	Q(4111)	Q(4030)	Q(4003)	Q(4021)	Q(4012)	$\bar{Q}(4)$				
0.0625	0	0	0	0	0	0	0	0	0	0	0				
0.09	205.93	191.47	191.31	178.44	174.19	186.81	159.56	150.86	183.02	181.92	183.23				
0.125	287.24	296.70	297.26	287.27	293.99	296.72	278.80	256.80	287.67	275.46	288.57				
0.16	297.21	320.69	320.66	340.48	340.41	322.97	329.00	297.14	327.63	326.31	322.81				
0.36	196.14	225.57	226.02	248.68	248.09	232.33	250.45	221.47	227.94	212.08	229.10				
0.64	121.26	137.97	142.62	154.90	161.82	147.31	171.32	145.39	145.07	135.20	145.55				
1.0	81.209	91.937	96.442	104.97	111.17	87.031	118.93	100.43	93.022	92.038	96.871				

Table V. Cross sections in units of  $\pi a_0^2$  for the ionization of the hydrogen atom in  $n = 5$  level by electron collision, calculated in the Born approximation and employing the parabolic coordinates. The cross section of each sublevel is designated by  $Q(n m n_1 n_2)$ . With the ten of the sublevel cross sections listed doubly degenerate, the list of the 25 components of  $n = 5$  level is complete.  $Q(5)$  is the averaged cross section for  $n = 5$  level.

Impact Energy ryd	eV	Q(5400)	Q(5310)	Q(5301)	Q(5220)	Q(5202)	Q(5211)	Q(5130)	Q(5103)	Q(5121)	Q(5112)	Q(5040)	Q(5004)	Q(5031)	Q(5013)	Q(5002)	Q(5)
		0.04		0	0	0	0	0	0	0	0	0	0	0	0	0	0
.0625	0.85	554.51	541.77	541.56	507.11	507.41	519.60	468.76	461.47	490.97	480.85	439.94	407.87	479.75	450.16	478.24	496.16
.09	1.22	735.85	783.02	777.15	834.33	791.10	695.04	806.21	805.70	804.00	803.31	763.77	673.70	794.08	716.97	744.84	774.59
.16	2.2	593.46	694.60	669.72	758.10	759.10	722.06	800.01	797.35	742.75	740.05	796.27	671.21	753.18	668.07	683.04	725.05
.36	4.9	320.68	358.11	365.11	408.30	408.45	387.71	447.88	420.16	386.89	375.03	470.25	318.11	412.40	339.78	362.09	386.37
.64	8.7	185.36	218.20	218.40	245.33	249.91	212.90	274.86	255.75	222.14	199.78	285.63	138.61	240.13	186.40	210.92	225.08
1.0	13.6	119.90	144.10	144.19	165.58	165.55	139.09	180.43	148.57	146.21	132.31	192.50	95.984	159.37	123.65	138.84	147.29

Table VI. Cross sections in units of  $\pi a_0^2$  for the ionization of the hydrogen atom in  $n = 6, 7, 8, 9, 10$  levels by electron collision, calculated in the Born approximation and employing the parabolic coordinates. For each level, the component with the greatest magnetic quantum number is computed. Since in parabolic coordinates all components of a given level have approximately equal values, the following table gives an indication of the cross section of the level considered.

Impact Energy		Q(6500)	Q(7600)	Q(8700)	Q(9800)	Q(10,900)
ryd	eV					
0.0121	0.16					3869
0.0144	0.20				3488	
0.0225	0.31			3651	7894	6367
0.0256	0.35		1286	4645		
0.0400	0.54	1135	2584	4483	6685	5064
0.0900	1.22	1326	1993	2794	3556	2748
0.1600	2.2	873	1288	1714	2121	1564
0.3600	4.9	448	608	788	990	725
0.6400	8.7	262	341	437	564	416
1.0000	13.6	170	227	290	362	268

Table VII. Ionization cross sections of hydrogen in  $n = 1, 2, 3, 4, 5$  levels by electron collision per unit energy range of the ejected electron.  $k_0^2$  is the energy of the incident electron and  $k^2$  is the energy of the ejected electron, both in rydberg units. The elements of each matrix are the averaged partial cross sections in units of  $\pi a_0^2/\text{ryd}$ .

a. $n = 1$										
$k_0^2 \backslash k^2$	0	1/256	1/64	1/16	1/4	9/16	1	9/4	4	25/4
1.0	0	0								
1.44	2.6148	2.5828	2.4881	2.1419	1.1175					
1.96	2.7376	2.7085	2.6235	2.3166	1.4642	0.72071				
2.00	2.7304	2.7014	2.6169	2.3121	1.4667	0.73398				
2.56	2.5614	2.5350	2.4578	2.1796	1.4150	0.77583	0.37420			
3.24	2.3216	2.2976	2.2277	1.9763	1.2886	0.72091	0.37786			
4.00	2.0844	2.0627	1.9995	1.7724	1.1537	0.64715	0.34517	0.09409		
6.25	1.5942	1.5772	1.5277	1.3502	0.87048	0.48371	0.25764	0.07860	0.02710	
9.00	1.2473	1.2337	1.1941	1.0525	0.67209	0.36901	0.19443	0.05890	0.02160	0.00903
b. $n = 2$										
$k_0^2 \backslash k^2$	0	1/256	1/64	1/16	1/4	9/16	1	9/4	1	25/4
0.25	0	0	0	0						
0.36	185.57	176.71	153.00	81.580						
0.50	181.29	173.99	154.36	99.479						
0.64	163.10	156.70	139.50	91.868	25.550					
1.00	124.59	119.67	106.49	70.321	21.952	6.2833				
1.44	96.202	92.338	81.996	53.796	16.729	5.2963	1.7677			
3.24	51.072	48.929	43.214	27.835	8.3166	2.6025	0.98032	0.21475		
5.29	34.098	32.631	28.731	18.310	5.3338	1.6404	0.61314	0.13612	0.04431	
7.29	26.044	24.907	21.888	13.858	3.9717	1.2085	0.44913	0.09937	0.03261	0.01334

Table VII (continued)

c. n = 3								
$k_0^2 \backslash k^2$	0	1/256	1/64	1/16	1/4	9/16	1	9/4
0.11	0	0	0					
0.16	2241.0	2008.2	1438.2					
0.22	2149.2	1962.4	1365.6	610.43				
0.36	1638.6	1501.0	1175.1	534.86				
0.64	1068.1	976.72	761.47	346.41	60.976			
1.00	740.07	672.27	522.27	234.56	40.253	9.5063		
4.00	226.90	203.61	154.30	64.973	10.047	2.2718	0.7043	0.0987
d. n = 4								
$k_0^2 \backslash k^2$	0	1/256	1/64	1/16	1/4	9/16		
0.0625	0	0	0					
0.09	12978	10597	5494.2					
0.125	12418	10529	6758.3					
0.16	10904	9337.0	6164.5	1688.2				
0.36	5948.9	5061.3	3344.9	1048.1	101.79			
0.64	3655.4	3106.2	2032.4	627.86	68.228	7.7489		
1.00	2481.0	2096.1	1358.9	407.37	42.138	7.9390		
e. n = 5								
$k_0^2 \backslash k^2$	0	1/256	1/64	1/16	1/4	9/16		
0.04	0	0	0					
0.0625	49804	37189	13924					
0.09	46099	35829	18886					
0.16	31466	24743	13604	2977.0				
0.36	15768	12181	6498.2	1414.6	105.37			
0.64	9415.8	7087.4	3705.6	794.02	60.879	6.8241		
1.00	6303.3	4711.1	2437.5	505.32	38.238	5.1182		

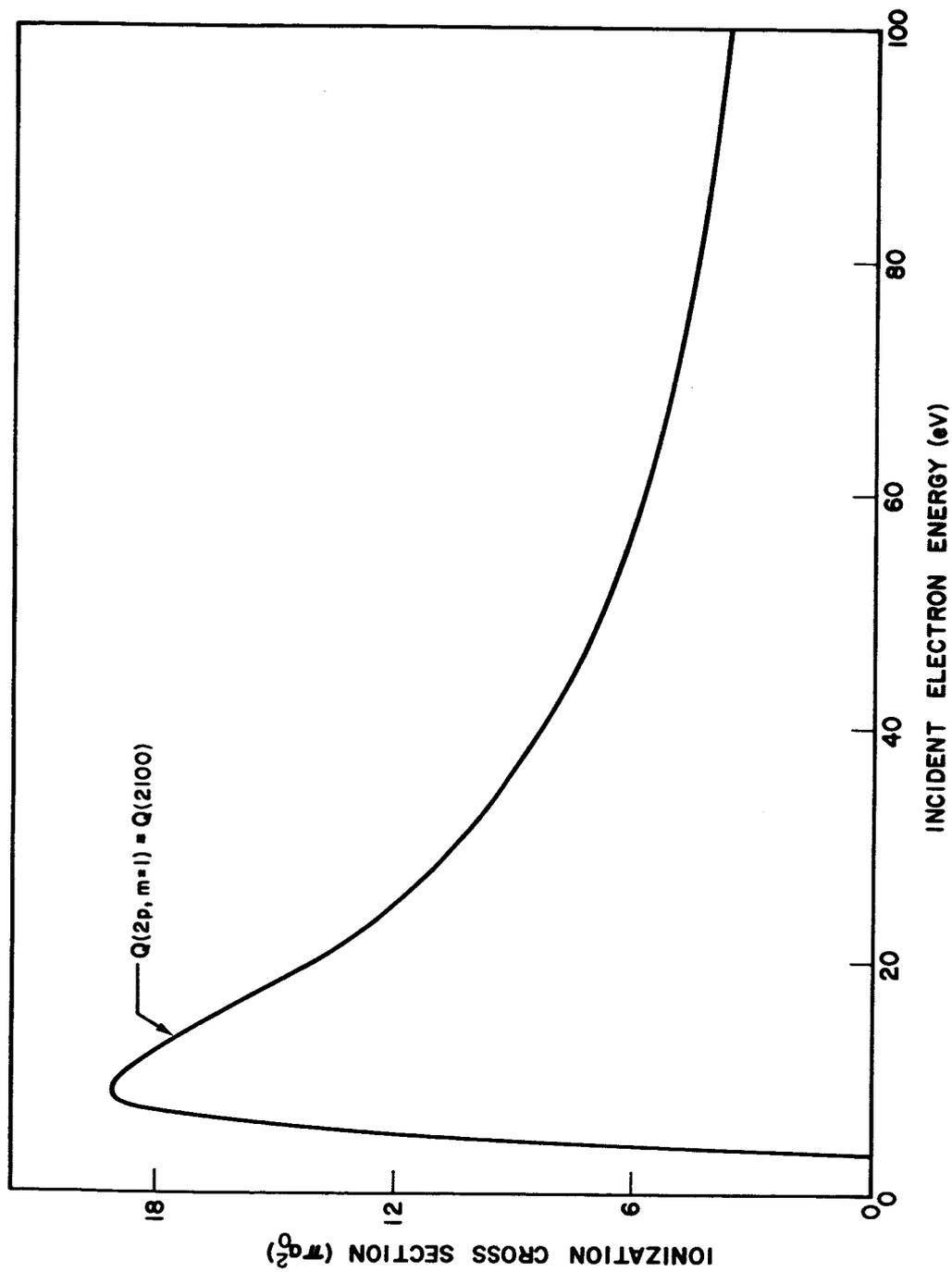


Fig. 1. Ionization cross section of the hydrogen in the  $2p, m = 1$  states.  $Q(2p, m = 1)$  and  $Q(2100)$  are the cross sections in spherical and parabolic coordinates respectively. Theoretically these two cross sections should be equal.

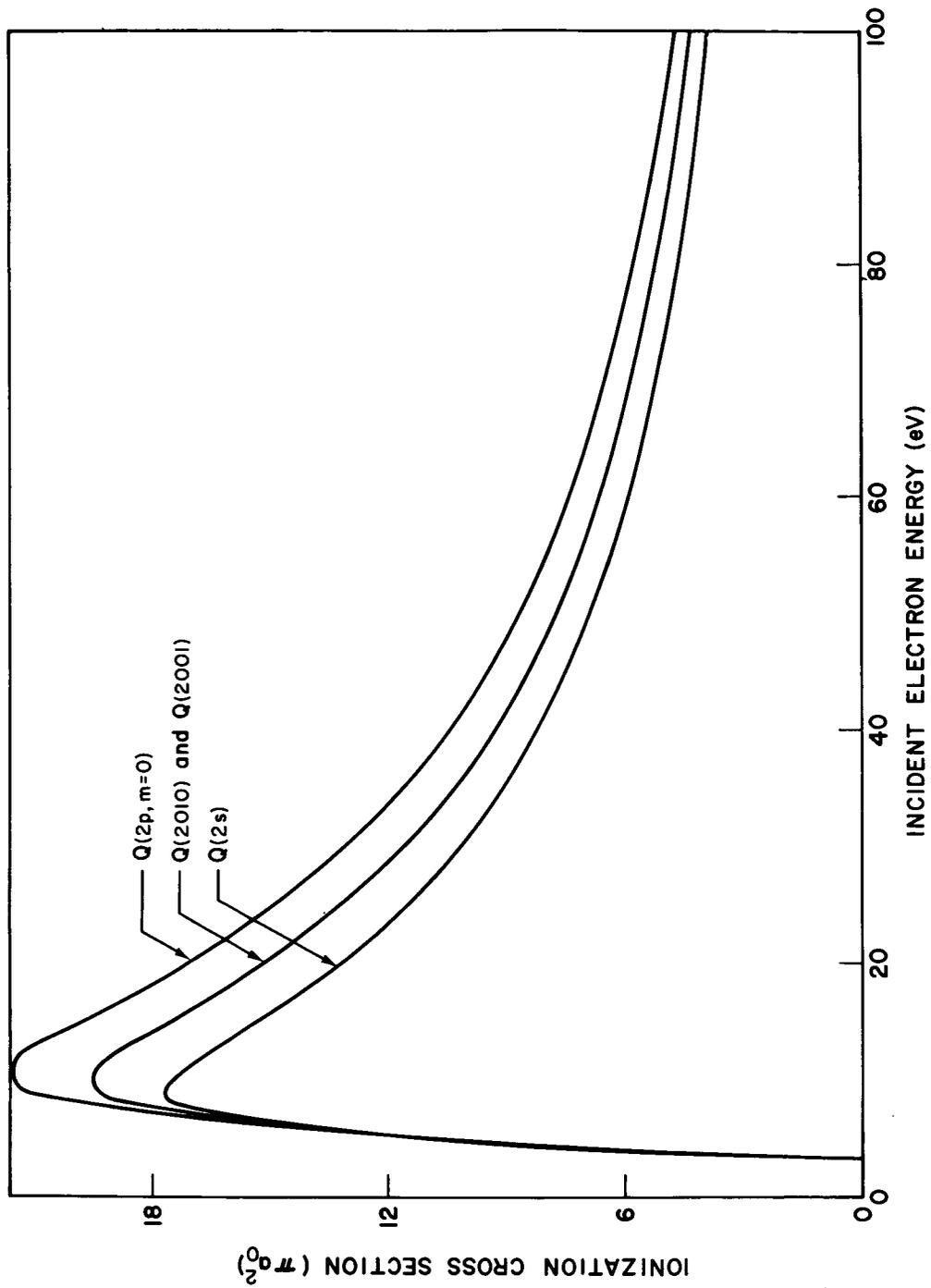


Fig. 2. Ionization cross section of the hydrogen in the 2s and the 2p,  $m = 0$  states. Theoretically the sum of the cross sections in spherical coordinates,  $Q(2s) + Q(2p, m = 0)$ , should be equal to the same sum in parabolic coordinates,  $Q(2010) + Q(2001)$ .

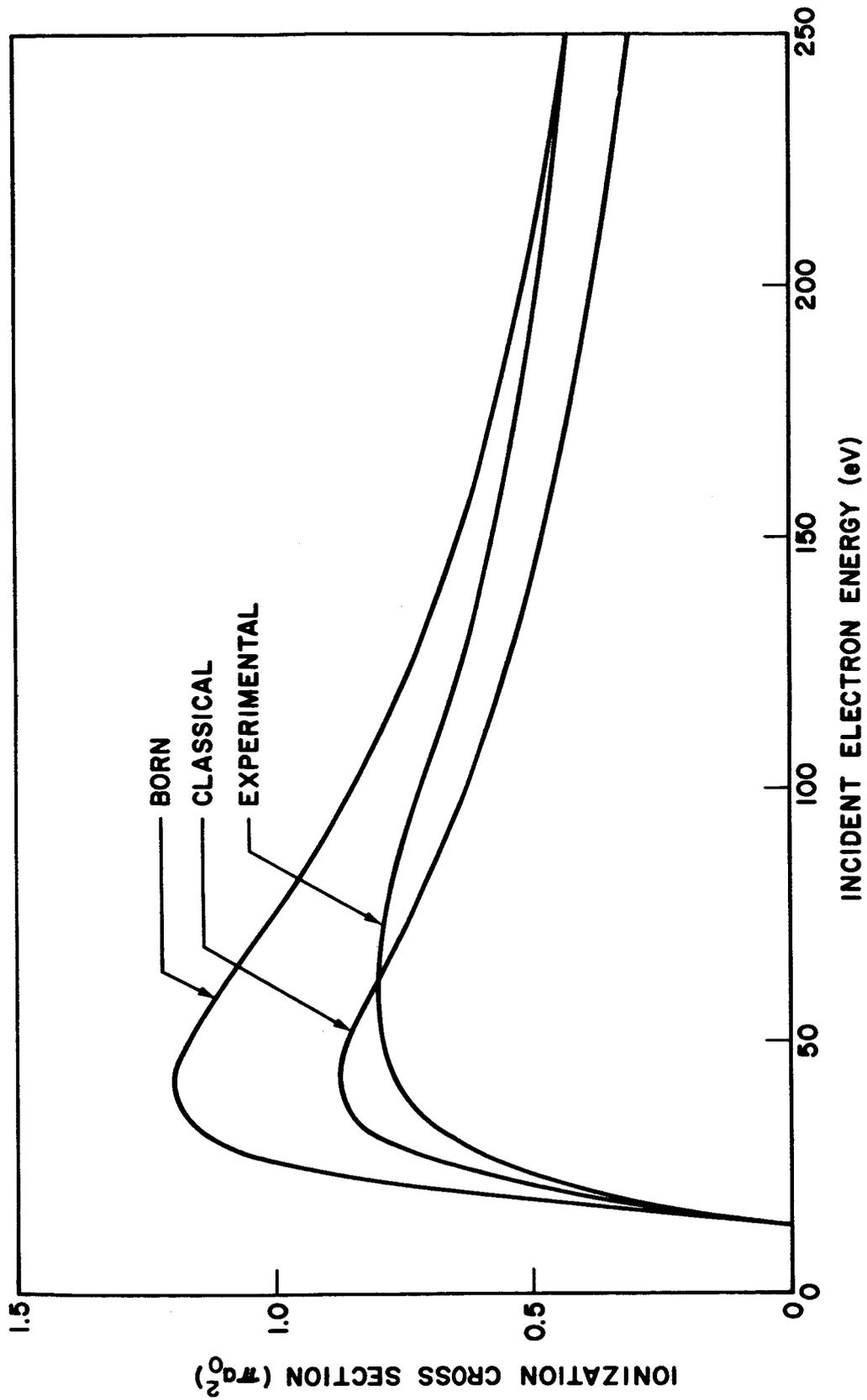


Fig. 3. Ionization of the ground state of the hydrogen. The theoretical curves, Born and classical, are compared with experimental curve.

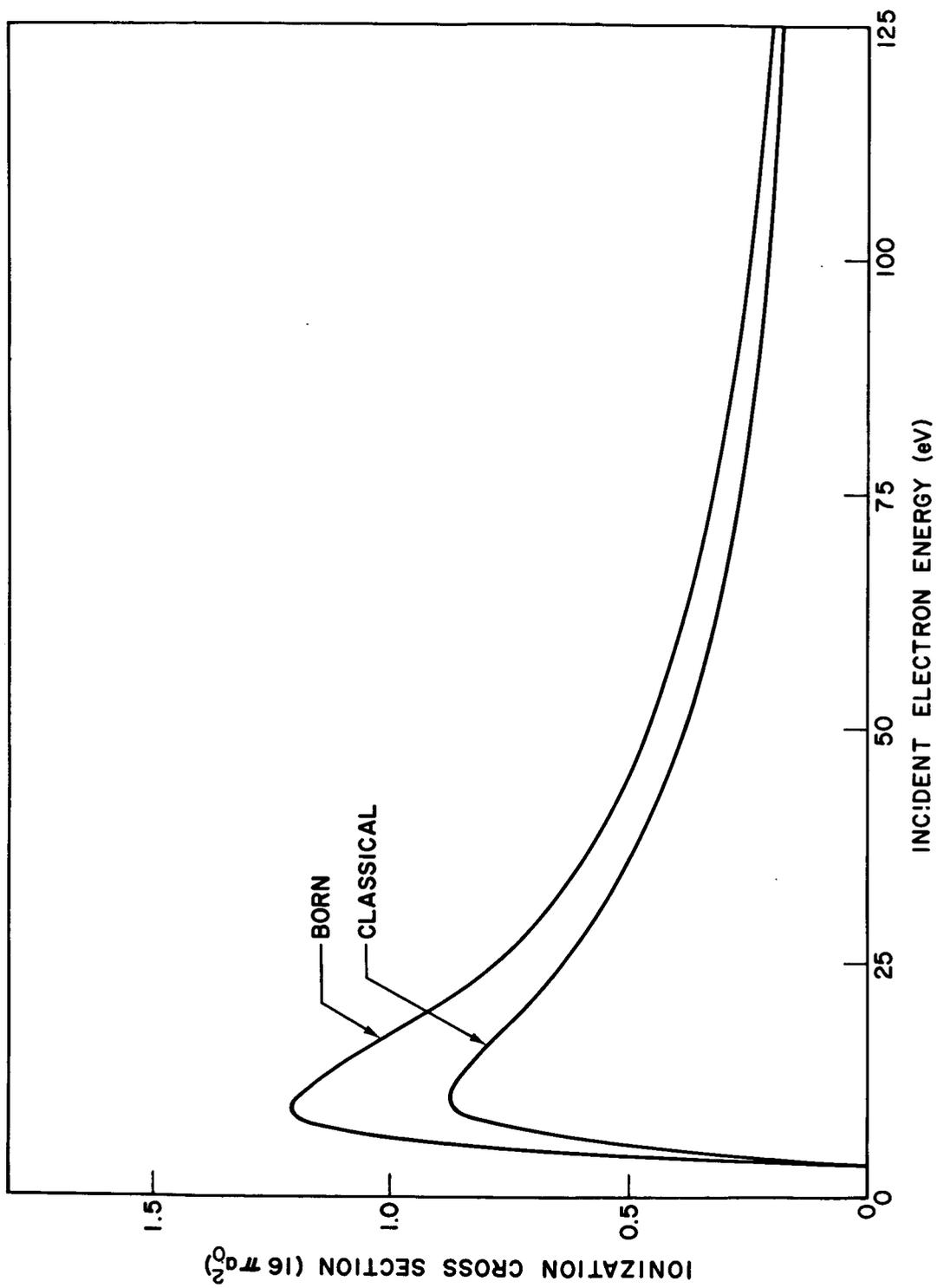


Fig. 4. Ionization of the hydrogen in the  $n = 2$  level.

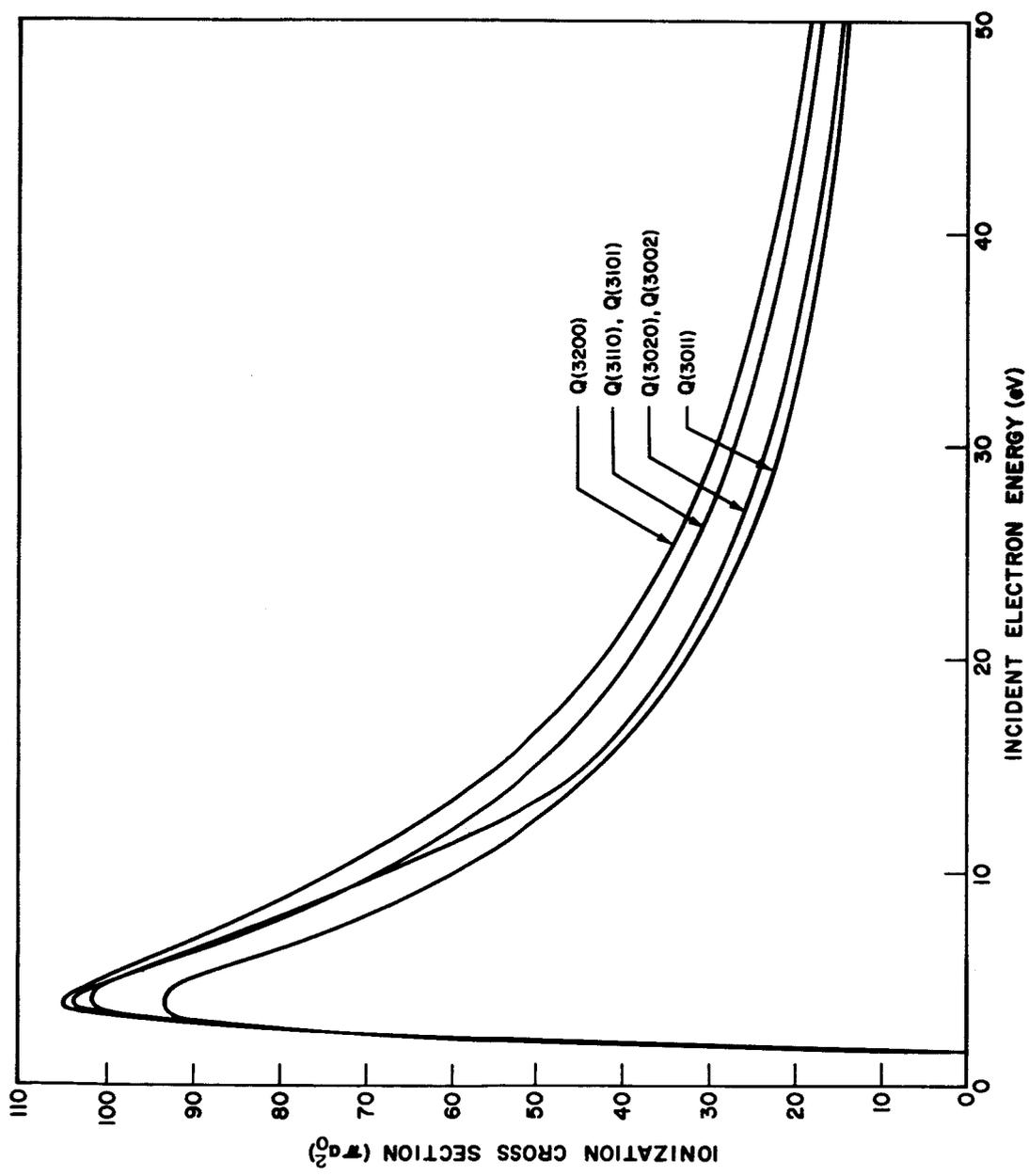


Fig. 5. Ionization of the hydrogen when the atom is in each of the sublevels of the level  $n = 3$ .  $Q(nm_1n_2)$  is the cross section corresponding to the initial state  $nm_1n_2$ .

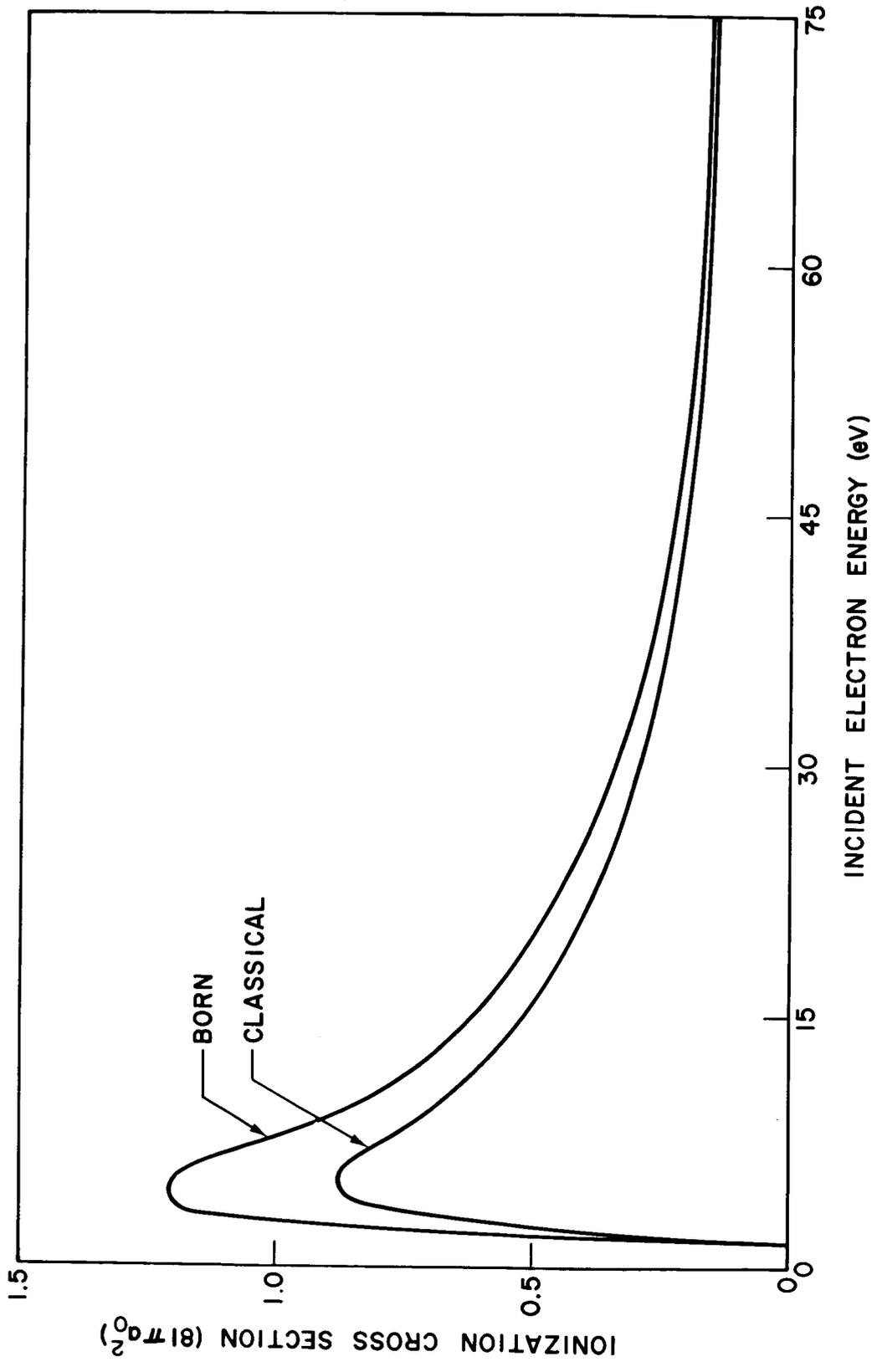


Fig. 6. Ionization of the hydrogen in the n = 3 level.

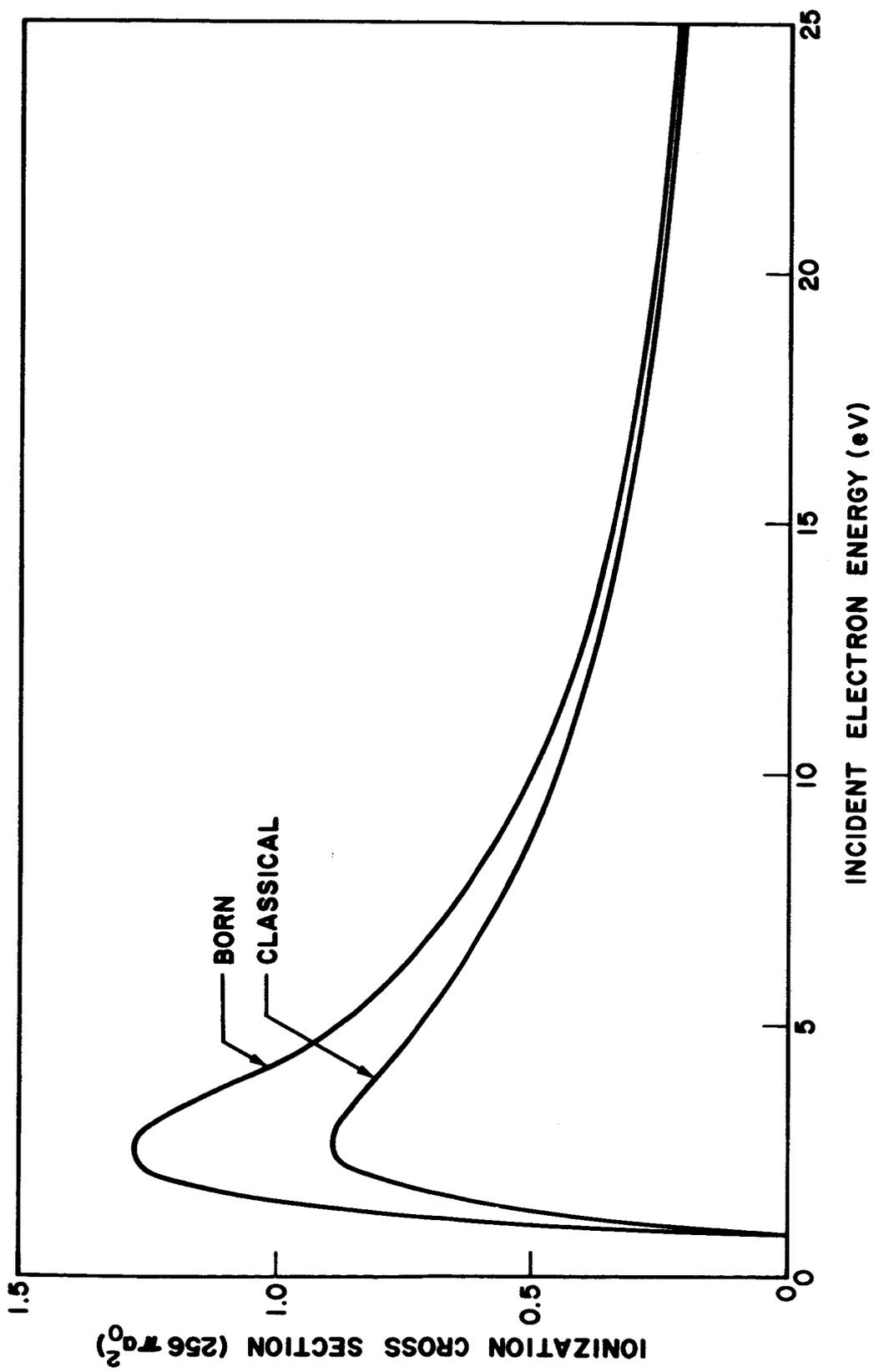


Fig. 7. Ionization of the hydrogen in the n = 4 level.

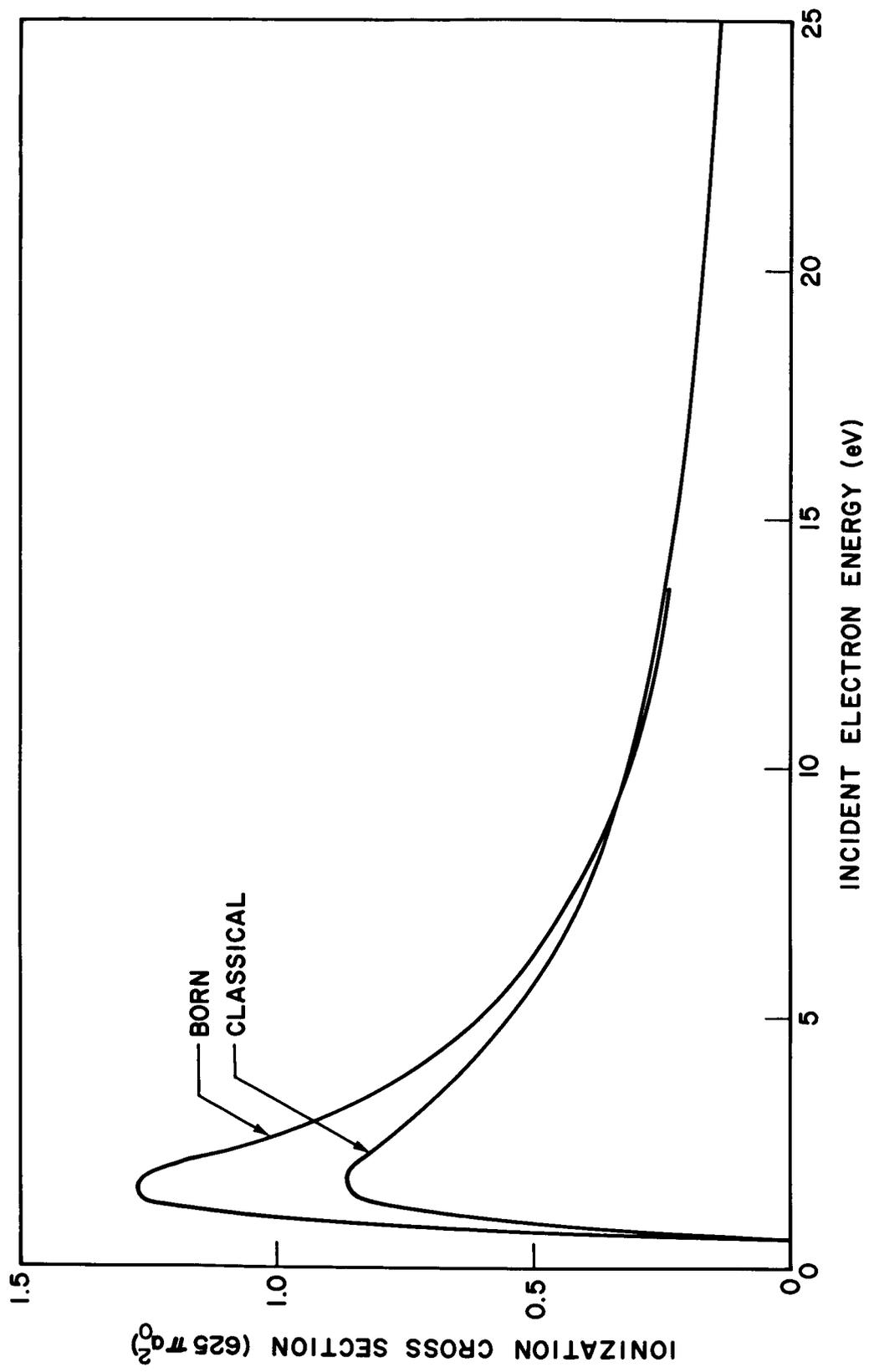


Fig. 8. Ionization of the hydrogen in the  $n = 5$  level.

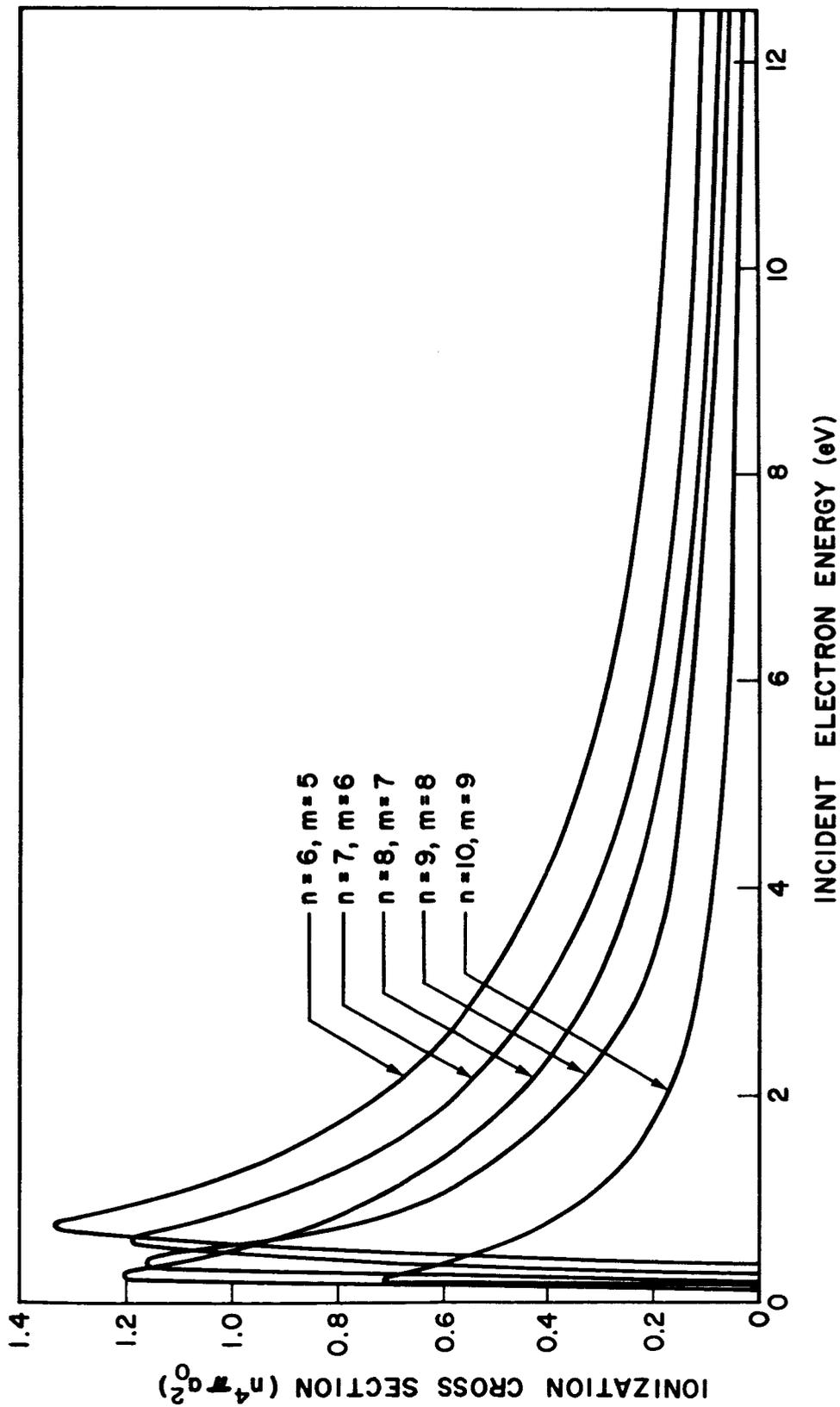


Fig. 9. Ionization of the hydrogen atom in the states  $n = 6, m = 5; n = 7, m = 6; n = 8, m = 7; n = 9, m = 8; n = 10, m = 9$ .

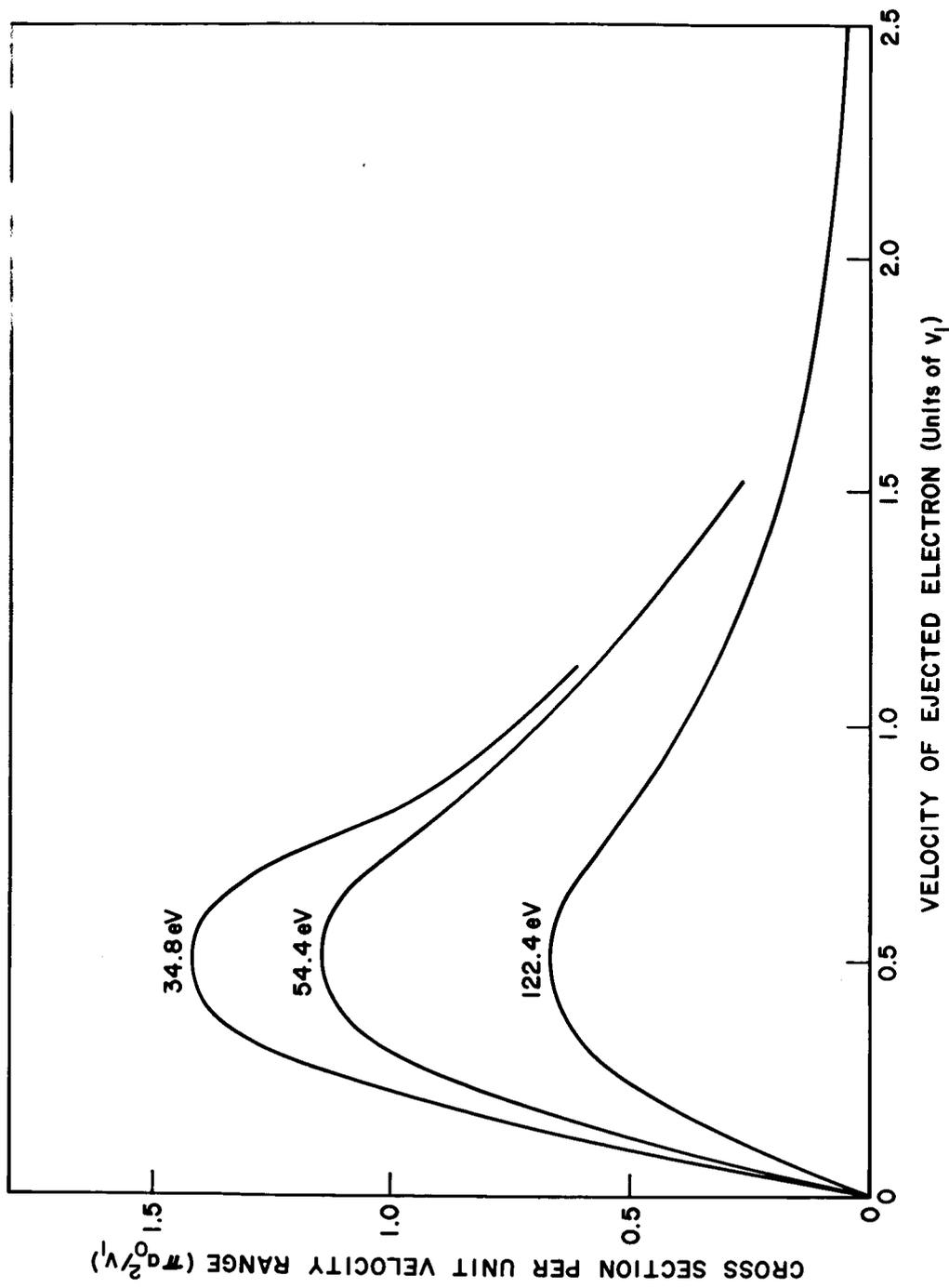


Fig. 10. Ionization cross section of the hydrogen in the  $n = 1$  level per unit velocity range of the ejected electron.  $V_1$  is velocity of the electron before ejection, i.e., the averaged velocity of the electron in the ground state of the hydrogen atom.

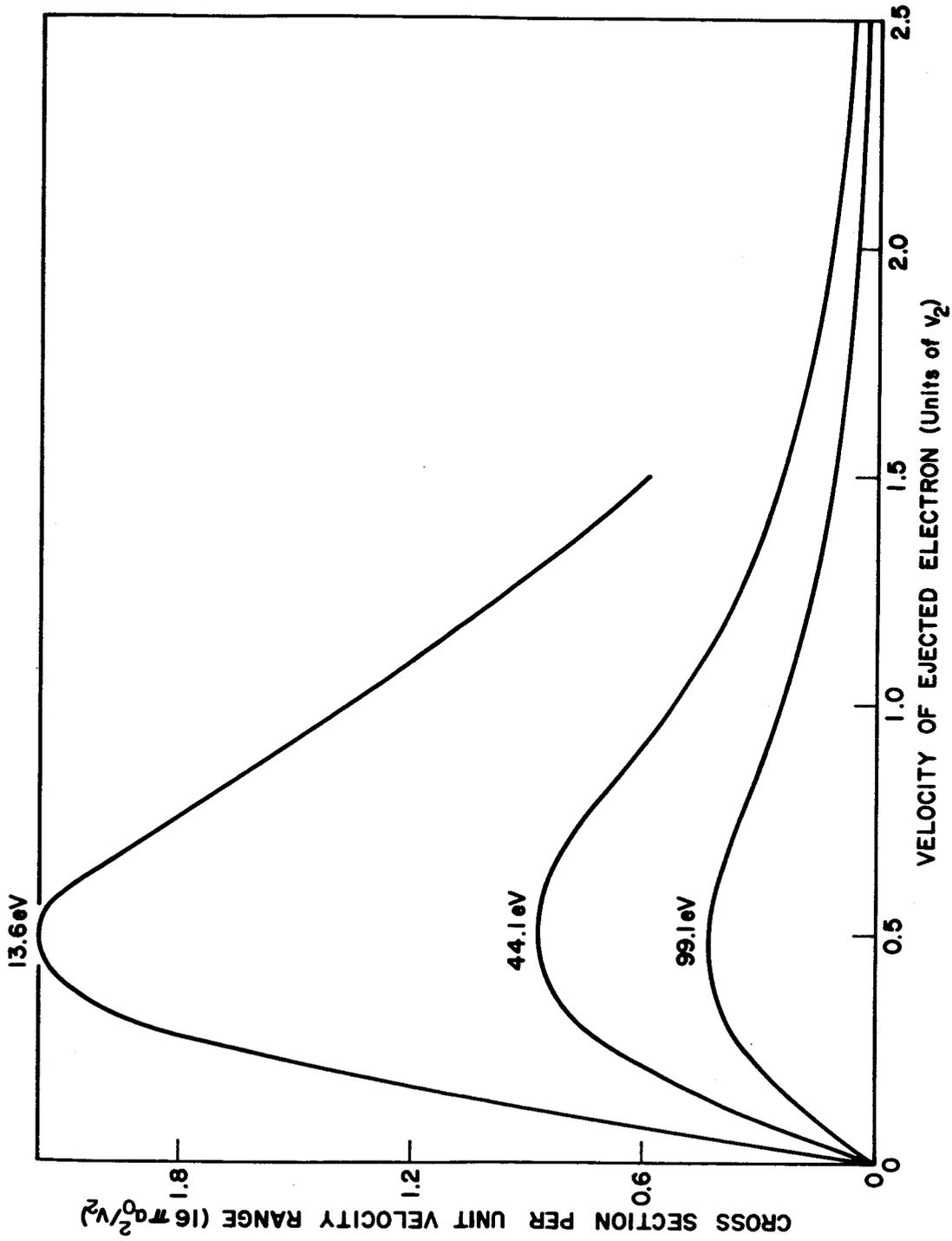


Fig. 11. Ionization cross section of the hydrogen in the  $n = 2$  level per unit velocity range of the ejected electron.  $v_2$  is the averaged velocity of the electron in the  $n = 2$  level of the hydrogen.

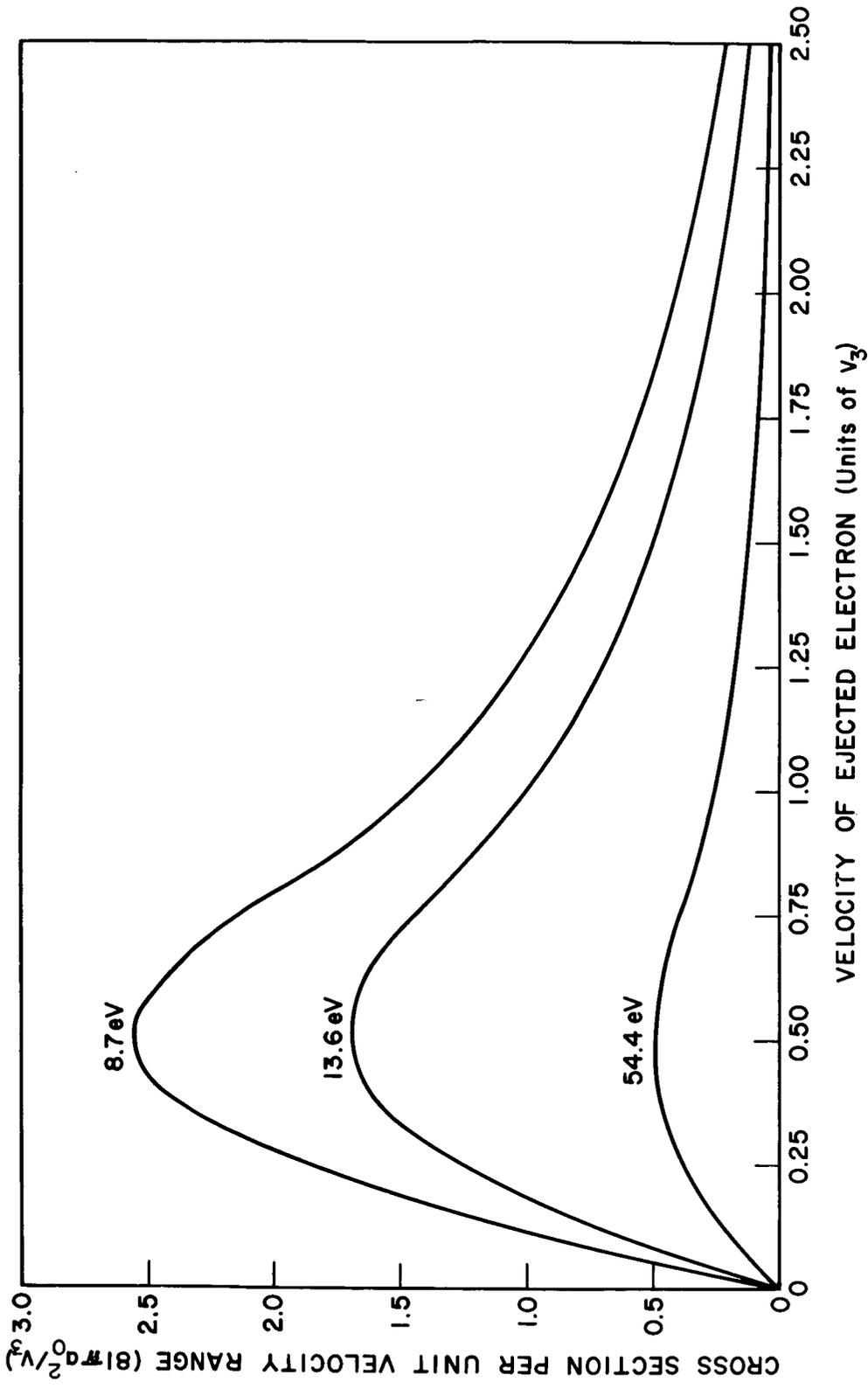


Fig. 12. Ionization cross section of the hydrogen in the  $n = 3$  level per unit velocity range of the ejected electron.  $v_3$  is the averaged velocity of the electron in the  $n = 3$  level of the hydrogen.

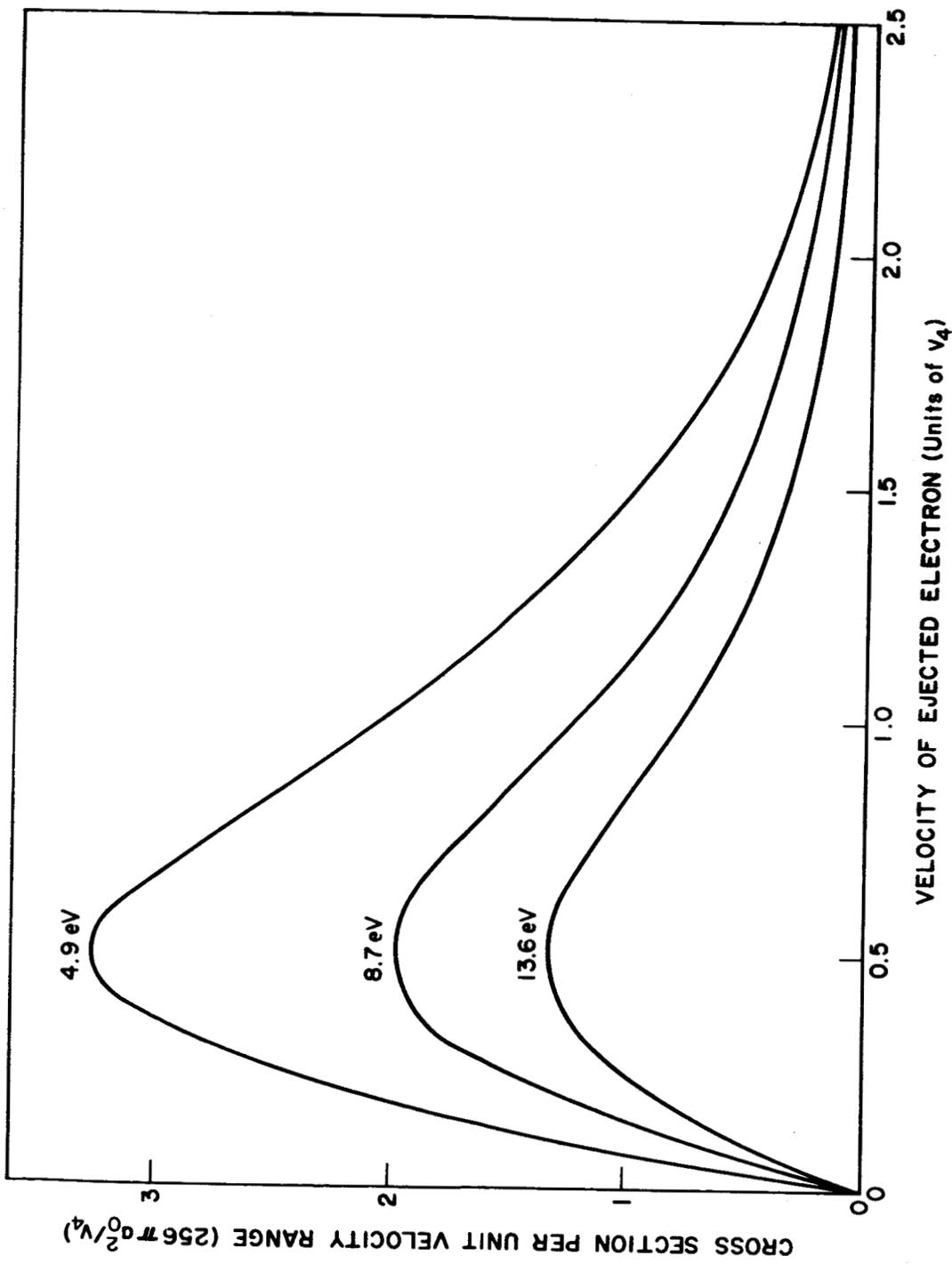


Fig. 13. Ionization cross section of the hydrogen in the  $n = 4$  level per unit velocity range of the ejected electron.  $v_4$  is the averaged velocity of the electron in the  $n = 4$  level of the hydrogen.

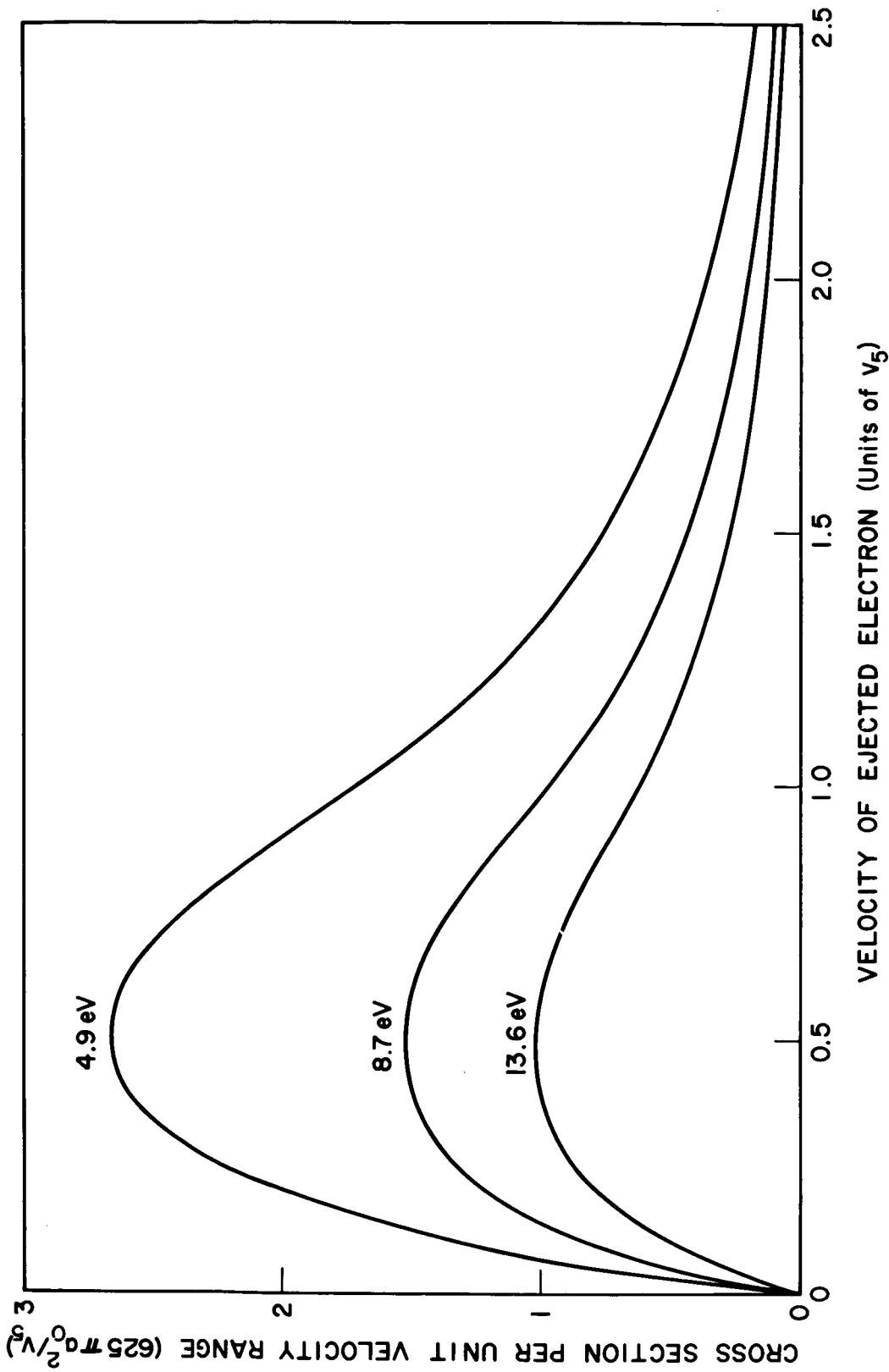


Fig. 14. Ionization cross section of the hydrogen in the  $n = 5$  level per unit velocity range of the ejected electron.  $V_5$  is the averaged velocity of the electron in the  $n = 5$  level of the hydrogen.