# Ionization of Excited Atomic Hydrogen by Electron Collision

KAZEM OMIDVAR

Laboratory for Theoretical Studies,\* Goddard Space Flight Center, National Aeronautics and Space Administration, Greenbelt, Maryland (Received 28 August 1964; revised manuscript received 18 February 1965)

A general formula in the Coulomb Born approximation is derived for ionization of the hydrogen atom by electron collision when the atom is in any given initial state. Using this formula, calculations are made for 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. In addition, the ionization cross section of one substate from each of the principal quantum numbers n=6, 7, 8, 9, 10 are calculated. The tabulated results cover the range of energies of interest in plasma calculations. Although the ionization amplitude is given in parabolic coordinates, the ionization cross section for a particular angular momentum of the atom can be obtained by a transformation of the ionization amplitude to spherical coordinates. Comparisons with experiment and other available theories are given.

## I. INTRODUCTION

PART from its purely theoretical interest, ionization is one of the main atomic processes in stellar atmospheres. This process occurs also in gas discharges and in plasmas. While electron-impact ionization is the dominant process for highly excited states of atomic hydrogen rather than photoionization, the former cross section is known with less accuracy than the latter. In this paper we calculate the cross section due to electron collision in the Born approximation. Because of practical difficulties in the measurement of the ionization cross section of the excited states, the calculated values remain the only source for application.

We review briefly the developments of the theoretical and experimental work on this particular form of ionization. The classical value of the ionization cross section with the atom in any initial state was calculated by Thomson.<sup>1</sup> Massey and Mohr<sup>2</sup> calculated, within the Born approximation, the ground-state ionization of the hydrogen atom. Burhop,<sup>3</sup> extending the same technique, formulated the ionization from substates of the first excited state without giving any numerical results for the case of hydrogen. Yavorsky4 has given the ionization for all s states of hydrogen in the form of a triple sum and a triple integration. The results for 2s and 3s states are shown graphically in his paper. Mandl,<sup>5</sup> rederiving the equations of Burhop, has given the results of ionization from the 2p,  $m = \pm 1$  states, again in graphical form. Later Swan,<sup>6</sup> taking the equations of Burhop, has carried out the numerical integrations, which are tabulated for the states 2s, 2p,  $m=0, \pm 1$ . In addition to a mistake of a factor of 2, the numerical integration in this paper does not appear very accurate.

Outside of the Born approximation, Geltman<sup>7</sup> 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.

The first measurement of the ionization of hydrogen by electrons was made by Fite and Brackmann.<sup>8</sup> They showed that the measurement agrees with the Born approximation beyond 100 eV. This measurement was followed by those of Boyd and Boksenberg,9 and Rothe et al.10

Among other theoretical works of interest are the inclusion of exchange in ionization by Peterkop,<sup>11</sup> treatments of the ionization in the impulse approximation by Akerib and Borowitz12 and in the close-coupling approximation by Taylor and Burke,13 and derivation of the threshold law for ionizing collisions by Rudge and Seaton.14

The Born approximation consists in representing the ionizing electron by a plane wave, the bound electron by a hydrogenic wave function, and the ejected electron by a Coulomb wave function. Physically, this means 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. This approximation also involves the exclusion of two less important effects: the exchange of the two electrons, and the effect of the

<sup>1960</sup>), Vol. 1, p. 529. <sup>10</sup> E. W. Rothe, L. L. Marino, R. H. Neynaber, and S. M. Trujillo, Phys. Rev. **125**, 582 (1962).

<sup>11</sup> R. Peterkop, Proc. Phys. Soc. (London) 77, 1220 (1961).

<sup>12</sup> R. Akerib and S. Borowitz, Phys. Rev. **122**, 1177 (1961). Some calculations in this paper are in error (private communication with

 <sup>13</sup> A. J. Taylor and P. G. Burke, Proceedings of the Third International Conference on Atomic Collisions, edited by M. R. C. McDowell (North-Holland Publishing Company, Amsterdam, 2000) <sup>14</sup> M. R. H. Rudge and M. J. Seaton, Proc. Phys. Soc. (London)

83, 680 (1964); Proc. Roy. Soc. (London) A283, 262 (1965).

<sup>\*</sup> Formerly The Theoretical Division.

<sup>&</sup>lt;sup>1</sup> J. J. Thomson, Phil. Mag. 23, 449 (1912).

<sup>&</sup>lt;sup>2</sup> H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) A140, 613 (1933).

<sup>&</sup>lt;sup>3</sup> E. H. S. Burhop, Proc. Cambridge Phil. Soc. 36, 43 (1940).

<sup>&</sup>lt;sup>4</sup> B. Yavorsky, Compt. Rend. Acad. Sci. U.R.S.S. 49, 250 (1945).

<sup>&</sup>lt;sup>6</sup> F. Mandl, The Ionization by Electron Impact of Excited Hydrogen Atoms (Atomic Energy Research Establishment, Harwell, England, 1952).

<sup>&</sup>lt;sup>6</sup> P. Swan, Proc. Phys. Soc. (London) A68, 1157 (1955).

<sup>&</sup>lt;sup>7</sup> S. Geltman, Phys. Rev. 102, 171 (1956).
<sup>8</sup> W. L. Fite and R. T. Brackmann, Phys. Rev. 112, 1141 (1958).
<sup>9</sup> R. L. F. Boyd and A. Boksenberg, *Proceedings of the 4th International Conference on Ionization Phenomena in Gases*, Uppsala, 1959 (North-Holland Publishing Company, Amsterdam, 1960).

polarization of the atom by the incident electron. The exchange effect can easily be included in the Born approximation. This will be the subject of a later paper.

With the nucleus fixed, the total ionization cross section involves twelve integrals: six over the spatial coordinates and the other 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> Cf the remaining eleven integrations, nine are carried out analytically, and 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, although it can be obtained by a unitary transformation of the ionization amplitude before the integration is carried out to find the total cross section.

The outline of the method is as follows. With  $\psi_i$  and  $\psi_f$  the initial and the final wave functions, the ionization or excitation amplitudes are proportional to the expression

$$V(K) = \int e^{iKz} \psi_i^* (\mathbf{r}) \psi_f(\mathbf{r}) d^3 r , \qquad (I.1)$$

known as the atomic form factor.  $\psi_f$  is a Coulomb wave function for the case of ionization. For the hydrogenic wave functions we can write

$$\psi_{i}(\mathbf{r}) = \exp[\alpha_{i}(\xi+\eta)]u_{i}(\xi)v_{i}(\eta),$$
  

$$\psi_{f}(\mathbf{r}) = \exp[\alpha_{f}(\xi+\eta)]u_{f}(\xi)v_{f}(\eta),$$
(I.2)

with  $\alpha_i$  and  $\alpha_f$  some constants, and  $u_i$ ,  $u_f$ ,  $v_i$ , and  $v_f$  some known analytic functions. Remembering that  $z = \frac{1}{2}(\xi - \eta)$  and  $d^3r = \frac{1}{4}(\xi + \eta)d\xi d\eta$ , Eq. (I.1) may be written

$$V(K) = \partial W / \partial c , \qquad (I.3)$$

where

$$c = \alpha_i^* + \alpha_f, \qquad (I.4)$$

$$W(K) = \frac{1}{4} \int_{0}^{\infty} \exp\left\{\left[c + \frac{iK}{2}\right]\xi\right\} u_{i}^{*}(\xi)u_{f}(\xi)d\xi$$
$$\times \int_{0}^{\infty} \exp\left\{\left[c - \frac{iK}{2}\right]\eta\right\} v_{i}^{*}(\eta)v_{f}(\eta)d\eta. \quad (I.5)$$

It is enough to evaluate the first integral, as the second one is similar to the first. Assume that  $G_1(\xi,s)$ ,  $G_2(\xi,t)$  are the generating functions of  $u_i(\xi)$  and  $u_f(\xi)$ ,

$$G_1(\xi,s) = \sum_{i=0}^{\infty} u_i(\xi) s^i, \quad G_2(\xi,t) = \sum_{f=0}^{\infty} u_f(\xi) t^f; \quad (I.6)$$

it follows that

$$\sum_{k=0}^{\infty} \sum_{f=0}^{\infty} s^{i} t^{f} \int_{0}^{\infty} \exp\left\{\left[c + \frac{iK}{2}\right]\xi\right\} u_{i}(\xi) u_{f}(\xi) d\xi$$
$$= \int_{0}^{\infty} \exp\left\{\left[c + \frac{iK}{2}\right]\xi\right\} G_{1}(\xi, s) G_{2}(\xi, t) d\xi. \quad (I.7)$$

By using the closed forms of  $G_1(\xi,s)$  and  $G_2(\xi,t)$ , the right-hand side of this equation can be evaluated. Suppose it is equal to S(s,t). If a Taylor's expansion of S(s,t) is made with respect to s and t, we obtain

$$\int_{0}^{\infty} \exp\left\{\left[c + \frac{iK}{2}\right]\xi\right\} u_{i}(\xi)u_{f}(\xi)d\xi = (i!f!)^{-1}\frac{\frac{\partial^{i+f}}{\partial S}(0,0)}{\partial s^{i}\partial t^{f}}, \quad (I.8)$$

which is the desired analytic expression. Similarly, the second factor on the right of (I.5) can be evaluated and V(K) determined.

#### **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

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

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 excitation or ionization amplitudes are proportional to

$$V(K) = \int \exp[iKz] \psi_i^*(\mathbf{r}) \psi_f(\mathbf{r}) d^3r , \qquad \text{(II.2)}$$

where

$$\mathbf{K} = \mathbf{k}_0 - \mathbf{k}_1, \qquad (II.3)$$

and  $\psi_i$  and  $\psi_f$  are the initial and final wave functions. The excitation cross section is given by<sup>16</sup>

$$Q_{e} = \frac{8\pi}{a_{0}^{2}k_{0}^{2}} \int_{k_{0}-k_{1}}^{k_{0}+k_{1}} |V(K)|^{2} \frac{dK}{K^{3}}, \qquad (\text{II.4})$$

with  $a_0$  the Bohr radius. In the case of ionization an additional integration should be performed over the final states of the ejected electron. Let k,  $\theta_k$ ,  $\phi_k$  be the polar coordinates of the ejected electron propagation vector **k** with respect to **K** as the *z* axis. The expression for the

<sup>&</sup>lt;sup>15</sup> The conservation of momentum is given up as the price of neglecting the motion of the nucleus.

<sup>&</sup>lt;sup>16</sup> H. S. Massey, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 36, Sec. 18.

cross section becomes

$$Q_{i} = \frac{8\pi}{a_{0}^{2}k_{0}^{2}} \int |V(\mathbf{k},K)|^{2} \frac{d^{3}kdK}{K^{3}},$$

$$= \frac{8\pi}{a_{0}^{2}k_{0}^{2}} \int_{0}^{k_{\max}} \int_{-1}^{+1} \int_{0}^{2\pi} \int_{k_{0}-k_{1}}^{k_{0}+k_{1}} |V(\mathbf{k},K)|^{2} \times \frac{k^{2}dkdxd\phi_{k}dK}{K^{3}}, \quad (\text{II.5})$$

where

and

$$x = \cos \theta_k , \qquad (\text{II.6})$$

$$k_{\rm max}^2 = k_0^2 - (Z^2/a_0^2 n^2),$$
 (II.7)

with n the principal quantum number of the atom before ionization and Z the effective charge of the nucleus.

### 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>17,18</sup>

$$\phi_{n_1n_2m}(\xi,\eta,\phi) = N_{n_1n_2m} \exp\left[-\frac{1}{2}\alpha(\xi+\eta)\right](\xi\eta)^{m/2}$$

$$\times L^{m_{n_1+m}}(\alpha\xi)L^{m_{n_2+m}}(\alpha\eta) \cos m\phi;$$

$$\alpha = \frac{Z}{n}; \quad n_1, n_2, m = 0, 1, 2, 3, \cdots, \qquad \text{(II.8)}$$

with

$$N_{n_1 n_2 m} = \left(\frac{\epsilon_m}{2\pi}\right)^{1/2} \left(\frac{2}{n}\right)^{1/2} \times \frac{\alpha^{m+3/2} [n_1! n_2!]^{1/2}}{[(n_1+m)!(n_2+m)!]^{3/2}}, \quad (\text{II.9})$$
$$\epsilon_m = \begin{cases} 2, & m \neq 0\\ 1, & m = 0. \end{cases} \quad (\text{II.10})$$

Equation (II.8) 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. It is given bv19

$$\psi(\mathbf{k},\mathbf{r}) = \frac{1}{2\pi} \left[ \frac{\beta}{1 - \exp(-2\pi\beta)} \right]^{1/2} \frac{e^{ikr}}{\Gamma(1 - i\beta)}$$
$$\times \int_0^\infty e^{-u} u^{-i\beta} J_0(R) du, \quad (\text{II.11})$$
where
$$R = 2 \left[ iu(kr - \mathbf{k} \cdot \mathbf{r}) \right]^{1/2}, \qquad (\text{II.12})$$

with the appropriate asymptotic form

$$\psi(\mathbf{k},\mathbf{r})\sim(2\pi)^{-3/2}e^{ik\tau}.$$
 (II.13)

Substitution of (II.8) and (II.11) in (II.2) gives the ionization amplitude in parabolic coordinates,

$$V(\mathbf{k},K) = \frac{N_{n_1n_2m}}{2\pi} \left(\frac{\beta}{1-e^{-2\pi\beta}}\right)^{1/2} \frac{1}{4\Gamma(1+i\beta)} \int \int \int \int \exp\left[-\frac{1}{2}\alpha(\xi+\eta) + \frac{i}{2}K(\xi-\eta) - \frac{i}{2}k(\xi+\eta) - u\right]$$
  
If we write 
$$\times (\xi\eta)^{m/2} L^m{}_{n_1+m}(\alpha\xi) L^m{}_{n_2+m}(\alpha\eta) \cos(m\phi) u^{i\beta} J_0(R^*)(\xi+\eta) dud\xi d\eta d\phi. \quad (\text{II.14})$$

$$R^* = [\rho^2 + \sigma^2 - 2\rho\sigma \cos(\phi - \phi_k)]^{1/2}, \qquad (II.15)$$

where

$$\rho = 2(-iuk)^{1/2} \sin(\theta_k/2)(\xi)^{1/2},$$
  

$$\sigma = 2(-iuk)^{1/2} \cos(\theta_k/2)(\eta)^{1/2},$$
(II.16)

then  $R^*$ ,  $\rho$ , and  $\sigma$  can be considered to form a triangle, and by the addition theorem for the Bessel functions,<sup>20</sup>

$$J_0(R^*) = \sum_{n=0}^{\infty} \epsilon_n J_n(\rho) J_n(\sigma) \cos n(\phi - \phi_k), \qquad (\text{II.17})$$

where  $\epsilon_n$  is defined in (10), it follows that

$$\int_{0}^{2\pi} J_0(R^*) \cos m\phi d\phi = 2\pi J_m(\rho) J_m(\sigma) \cos m\phi_k.$$
(II.18)

<sup>17</sup> L. I. Schiff, Quantum Mechanics (McGraw-Hill Book Company, Inc., New York, 1949), 1st ed., Sec. 16.
 <sup>18</sup> H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One and Two Electron Atoms (Springer-Verlag, Berlin, 1957), Sec. 6.
 <sup>19</sup> A. Sommerfeld, Ann. Physik 11, 257 (1931).
 <sup>20</sup> G. N. Watson, Theory of Bessel Functions (Cambridge University Press, New York, 1958), 2nd ed., Sec. 4.82.

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Making use of Eq. (II.18) in Eq. (II.14) we can write

$$V(k,K,\theta_k,\phi_k) = \frac{1}{2\pi} \left( \frac{\beta}{1 - e^{-2\pi\beta}} \right)^{1/2} \cos(m\phi_k) I(mn_1n_2 | kK\theta_k),$$
(II.19)

where

$$I(mn_1n_2|kK\theta_k) = \frac{\pi N_{n_1n_2m}}{2\Gamma(1+i\beta)} \int \int \int \exp\left[-\frac{1}{2}(\alpha+ik)(\xi+\eta) + \frac{i}{2}K(\xi-\eta) - u\right] \times (\xi\eta)^{m/2} L^m_{n_1+m}(\alpha\xi) L^m_{n_2+m}(\alpha\eta) u^{i\beta} J_m(\rho) J_m(\sigma)(\xi+\eta) dud\xi d\eta. \quad (II.20)$$

The ionization cross section as given by Eq. (II.5), after integration with respect to  $\phi_k$ , can now be written ( $a_0 = 1$ ):

$$Q(nmn_1n_2) = \frac{2Z}{\pi k_0^2} \left(\frac{2\pi}{\epsilon_m}\right) \int_0^{k_{\max}} \int_{k_0-k_1}^{k_0+k_1} \int_{-1}^{+1} |I(mn_1n_2|kK\theta_k)|^2 \times \frac{kdkdKdx}{K^3(1-e^{-2\pi Z/k})}.$$
 (II.21)

Using the generating functions of the associated Laguerre functions and introducing

$$p = \frac{1}{2}\alpha + \frac{1}{2}ik, \quad q = -\frac{1}{2}iK,$$
 (II.22)

we see that

$$\sum_{n_{1},n_{2}} \frac{s^{n_{1}}}{(n_{1}+m)!} \frac{t^{n_{2}}}{(n_{2}+m)!} I(mn_{1}n_{2})$$

$$= \frac{1}{(1-s)^{m+1}} \frac{1}{(1-t)^{m+1}} \frac{\pi N_{n_{1}n_{2}m}}{2\Gamma(1+i\beta)} \int \int \int \exp\left[-p(\xi+\eta) - q(\xi-\eta) - u - \frac{\alpha\xi s}{1-s} - \frac{\alpha\eta t}{1-t}\right]$$

$$\times (\xi\eta)^{m/2} u^{i\beta} J_{m}(\rho) J_{m}(\sigma) (\xi+\eta) dud\xi d\eta = -\frac{1}{(1-s)^{m+1}} \frac{1}{(1-t)^{m+1}} \frac{\pi N_{n_{1}n_{2}m}}{2\Gamma(1+i\beta)} \frac{\partial U}{\partial \rho}, \quad (\text{II.23})$$
where

where

$$U = \int_0^\infty u^{i\theta} e^{-u} du \times \int_0^\infty J_m(\rho) \xi^{m/2} \exp\left[-(p+q) - \frac{\alpha s}{1-s}\right] \xi d\xi \times \int_0^\infty J_m(\sigma) \eta^{m/2} \exp\left[-(p-q) - \frac{\alpha t}{1-t}\right] \eta d\eta. \quad (\text{II.24})$$

U can be evaluated by means of an integral given by Watson,<sup>21</sup>

$$\int_{0}^{\infty} J_{m}(az) e^{-p^{2} z^{2}} z^{m+1} dz = \frac{a^{m}}{(2p^{2})^{m+1}} \exp\left[-\frac{a^{2}}{4p^{2}}\right].$$
(II.25)

By introducing

$$P = (\mathbf{p}+q) + \lfloor \alpha s/(1-s) \rfloor, \quad Q = (\mathbf{p}-q) + \lfloor \alpha t/(1-t) \rfloor, \quad (\text{II.26})$$

$$U = \left(\frac{-ik\sin\theta_k}{2}\right)^m \Gamma(m+1+i\beta) \times \frac{(PQ)^{i\beta}}{\left[PQ - ikQ\sin^2\frac{\theta_k}{2} - ikP\cos^2\frac{\theta_k}{2}\right]^{m+1+i\beta}}.$$
 (II.27)

By definition of Eqs. (II.26),

$$\frac{\partial U}{\partial p} = \frac{\partial U}{\partial P} + \frac{\partial U}{\partial Q} = \left(\frac{-ik\sin\theta_k}{2}\right)^m \Gamma(i\beta + 1 + m) \times \frac{(PQ)^{i\beta - 1}}{\left[PQ - ikQ\sin^2\frac{\theta_k}{2} - ikP\cos^2\frac{\theta_k}{2}\right]^{m+2+i\beta}} \times \left[\beta k \left(P^2\cos^2\frac{\theta_k}{2} + Q^2\sin^2\frac{\theta_k}{2}\right) - (m+1)PQ(P+Q-ik)\right]. \quad (\text{II.28})$$

<sup>&</sup>lt;sup>21</sup> See Ref. 20, Sec. 13.30.

Equations (II.23), with some modification in Eq. (II.28), can now be written

$$\sum_{n_{1}n_{2}} \frac{s^{n_{1}tn_{2}}I(mn_{1}n_{2})}{(n_{1}+m)!(n_{2}+m)!} = -\frac{\pi}{2} N_{n_{1}n_{2}m} \frac{(i\beta-m)!}{(i\beta)!} \left(\frac{-ik\sin\theta_{k}}{2}\right)^{m} \\ \times \left[(1-s)(1-t)PQ\right]^{-(m+3)} \left[1-ik\left(\frac{\sin^{2}(\theta_{k}/2)}{P} + \frac{\cos^{2}(\theta_{k}/2)}{Q}\right)\right]^{-(m+2+i\beta)} \\ \times \left\{(1-s)^{2}(1-t)^{2} \left[\beta k\left(P^{2}\cos^{2}\frac{\theta_{k}}{2} + Q^{2}\sin^{2}\frac{\theta_{k}}{2}\right) - (m+1)PQ(P+Q-ik)\right]\right\}. \quad (II.29)$$

## Expansion in Terms of s and t

Since  $I(mn_1n_2)$  is independent of s and t, we can regard it as the coefficient of expansion of the right-hand side of Eq. (II.29) 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 by

$$a = K - i\alpha, \quad a^* = K + i\alpha. \tag{II.30}$$

Then it follows that

$$P = -\frac{i}{2} \times \frac{(a^* - k) - (a - k)s}{1 - s}, \quad Q = \frac{i}{2} \times \frac{(a + k) - (a^* + k)t}{1 - t}.$$
 (II.31)

With these values of P and Q substituted in Eq. (II.29), the factors on the right-hand side of this equation having integer powers can be expanded by binomial expansion while those having complex powers can be expanded by Taylor's expansion. We obtain in this way<sup>22</sup>

$$\sum_{n_{1}n_{2}} \frac{s^{n_{1}l_{n_{2}}I}(mn_{1}n_{2})}{(n_{1}+m)!(n_{2}+m)!} = -\frac{\pi}{2} (4)^{m+3} N_{n_{1}n_{2}m} \frac{(i\beta+m)!}{(i\beta)!} \left(\frac{-ik}{2}\right)^{m} (1-x^{2})^{m/2} \\ \times \sum_{j_{1}=0}^{\infty} \sum_{j_{2}=0}^{\infty} \sum_{l_{1}=0}^{\infty} \sum_{l_{2}=0}^{\infty} \sum_{\mu_{1}=0}^{\infty} \sum_{\mu_{2}=0}^{2} \binom{m+2+j_{1}}{j_{1}} \binom{m+2+j_{2}}{j_{2}} (a^{*}-k)^{-(m+3+j)} (a-k)^{j_{1}} \\ \times (a+k)^{-(m+3+j_{2})} (a^{*}+k)^{j_{2}} [l_{1}!l_{2}!]^{-1} y^{l_{1}l_{2}} (0,0) A_{\mu_{1}\mu_{2}} \times s^{j_{1}+l_{1}+\mu_{1}} \times t^{j_{2}+l_{2}+\mu_{2}}, \quad (\text{II.32})$$

where

$$y^{l_{1}l_{2}}(0,0) = \sum_{\nu_{1}=0}^{l_{1}} \sum_{\nu_{2}=0}^{l_{2}} C(\nu_{1},l_{1})C(\nu_{2},l_{2}) \frac{(i\beta+m+1+\nu_{1}+\nu_{2})!}{(i\beta+m+1)!} (-k)^{\nu_{1}+\nu_{2}} \\ \times (a-a^{*})^{\nu_{1}+\nu_{2}} [(a^{*}-k)(a+k)]^{i\beta+m+2} (a-k)^{l_{1}-\nu_{1}} (a^{*}-k)^{-(l_{1}-\nu_{2})} \\ \times (a+k)^{-(l_{2}-\nu_{1})} (a^{*}+k)^{l_{2}-\nu_{2}} (1-x)^{\nu_{1}} (1+x)^{\nu_{2}} [aa^{*}+k^{2}-kx(a+a^{*})]^{-(m+2+\nu_{1}+\nu_{2})}, \quad (\text{II.33})$$

$$A_{\mu_1\mu_2} = B_{\mu_1\mu_2} + xC_{\mu_1\mu_2}, \qquad (II.34)$$

$$B_{\mu_{1}\mu_{2}} = -\frac{Z}{8}(-)^{\mu_{1}+\mu_{2}} \binom{2}{\mu_{1}} \binom{2}{\mu_{2}} [(a^{*}-k)^{2}e^{2i\mu_{1}\phi_{1}} + (a+k)^{2}e^{2i\mu_{2}\phi_{2}}] \\ -\frac{\alpha}{4}(m+1)(-)^{\mu_{1}+\mu_{2}}(a^{*}-k)(a+k)[\bar{\delta}(\mu_{1}\mu_{2},22) - \bar{\delta}(\mu_{1}\mu_{2},00)e^{-2i(\phi_{1}+\phi_{2})}]e^{2i(\mu_{1}\phi_{1}+\mu_{2}\phi_{2})}, \quad (\text{II.35})$$

$$C_{\mu_{1}\mu_{2}} = -\frac{Z}{8}(-)^{\mu_{1}+\mu_{2}} \binom{2}{\mu_{1}} \binom{2}{\mu_{2}} [(a^{*}-k)^{2}e^{2i\mu_{1}\phi_{1}} - (a+k)^{2}e^{2i\mu_{2}\phi_{2}}], \qquad (II.36)$$

$$\phi_1 = \tan^{-1} [\alpha/(k-K)], \quad \phi_2 = \tan^{-1} [\alpha/(k+K)], \quad 0 < \phi_1, \quad \phi_2 < \pi,$$
 (II.37)

$$\bar{\delta}(\mu_1\mu_2, n_1n_2) = \begin{bmatrix} 1 - \delta(\mu_1, n_1) \end{bmatrix} \begin{bmatrix} 1 - \delta(\mu_2, n_2) \end{bmatrix},$$
(II.38)

<sup>&</sup>lt;sup>22</sup> For details of this expansion see K. Omidvar, External Report X-641-64-192, Goddard Space Flight Center, Greenbelt, Maryland (unpublished).

 $\delta(\mu,n)$  being the Kronecker delta. The coefficients  $C(\nu,l)$  given in Eq. (II.33) are defined by the following recursion relationship and the initial values:

$$C(\nu,l) = (l-1+\nu)C(\nu,l-1) + C(\nu-1,l-1), \quad \nu \leq l;$$
(II.39)

$$C(0,l) = \delta(0,l); \quad C(1,1) = 1; \quad C(\nu,l) = 0 \quad \text{for} \quad \nu > l.$$
 (II.40)

The first few values of  $C(\nu, l)$  are given in Table I.

Equating coefficients of equal powers of s and t on both sides of Eq. (II 32), and neglecting a constant phase factor in the amplitude of ionization, the following expression for  $I(mn_1n_2)$  results:

$$I(mn_1n_2) = (2)^{m+5}\pi(n_1+m)!(n_2+m)!N_{n_1n_2m}(iZ+(m+1)k)^{-1}[(K^2+\alpha^2+k^2)^2-4k^2K^2]^{-1/2}e^{-\beta\phi_3}\sum_{\gamma}G(\gamma)H(\gamma), \quad (\text{II.41})$$

where

$$\phi_3 = \tan^{-1} [2\alpha k / (K^2 + \alpha^2 - k^2)], \quad 0 \leq \phi_3 < \pi,$$
 (II.42)

and  $\gamma$  stands for the set of 8 integers  $j_1 l_1 \nu_1 \mu_1 j_2 l_2 \nu_2 \mu_2$  which must satisfy the following relationships:

$$j_1 + l_1 + \mu_1 = n_1, \quad \nu_1 \leq l_1; j_2 + l_2 + \mu_2 = n_2, \quad \nu_2 \leq l_2.$$
(II.43)

The  $G(\gamma)$  and  $H(\gamma)$  are defined by

$$G(\gamma) = \binom{m+2+j_1}{j_1} \binom{m+2+j_2}{j_2} (l_1!l_2!)^{-1} C(\nu_1, l_1) C(\nu_2, l_2) (2i\alpha)^{\nu_1+\nu_2} \times \left[\prod_{\omega=1}^{m+1+\nu_1+\nu_2} (iZ+\omega k)\right] \binom{a+k}{a-k}^{\nu_1} \left(\frac{a^*-k}{a^*+k}\right)^{\nu_2} \exp 2i\left[(j_1+l_1)\phi_1+(j_2+l_2)\phi_2\right], \quad (\text{II.44})$$

$$H(\gamma) = (1 - x^2)^{m/2} (1 - x)^{\nu_1} (1 + x)^{\nu_2} [B(\mu_1 \mu_2) + xC(\mu_1 \mu_2)] [aa^* + k^2 - kx(a + a^*)]^{-(m+2+\nu_1+\nu_2)}.$$
(II.45)

When  $I(mn_1n_2)$  is substituted from Eq. (II.41) in Eq. (II.21), and  $N_{n_1n_2m}$  is eliminated, we obtain

$$Q(nmn_1n_2) = 2 \int_{k=0}^{k_{\max}} q(nmn_1n_2|k)kdk, \qquad (II.46)$$

$$q(nmn_1n_2|k) = \frac{\pi^{2^7}(2\alpha)^{2m+4}}{k_0^2} \times \frac{n_1!n_2!}{(n_1+m)!(n_2+m)!} \times \frac{1}{[Z^2 + (m+1)^2k^2][1 - e^{-2\pi Z/k}]} \times \int_{k_0-k_1}^{k_0+k_1} \frac{e^{-2Z\phi_3/k}dK}{K^3[(\alpha^2 + K^2 + k^2)^2 - 4k^2K^2]} \times S(k,K), \quad (\text{II.47})$$

where

$$S(k,K) = \int_{-1}^{+1} |\sum_{\gamma} G(\gamma)H(\gamma)|^2 dx$$
$$= \sum_{\gamma} \sum_{\gamma'} G(\gamma)G^*(\gamma') \int_{-1}^{+1} H(\gamma)H^*(\gamma')dx. \qquad (II.48)$$

 $q(nmn_1n_2|k)$  is the cross section per unit energy range of the ejected electron in rydbergs.

A glance at the form of  $H(\gamma)$  in Eq. (II.45) suggests that integration with respect to x in Eq. (II.48) can be carried out by elementary methods. This will not be shown here although the integration has been carried out for evaluation of the cross sections.

#### Symmetry Considerations

Equation (II.14) shows that when members of the pairs  $\xi$ ,  $\eta$ ; K, -K;  $n_1$ ,  $n_2$ ; and  $\sin\theta_k/2$ ,  $\cos\theta_k/2$  are inter-

changed,  $V(\mathbf{k},K)$  remains invariant. Since  $\xi$  and  $\eta$  are the variables of integrations, their interchange does not change  $V(\mathbf{k},K)$ . 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

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



FIG. 1. Ionization of the ground state of the hydrogen. The theoretical curves, Born and classical, are compared with the experimental curve.

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  $x \rightleftharpoons -x$ . Then the above integral is invariant under the interchanges  $K \rightleftharpoons -K$ ,  $n_1 \rightleftharpoons n_2$ . Bearing this in mind,

| TABLE 1. The $C(v,t)$ values. |   |     |     |     |    |   |  |  |  |  |
|-------------------------------|---|-----|-----|-----|----|---|--|--|--|--|
| ž                             | 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 |  |  |  |  |

comparison of Eqs. (II.5), (II.47) leads to the following equation:

 $S(n_2n_1|kK) = S(n_1n_2|k-K).$ 

A further symmetry exists with respect to k and K. It is evident from Eqs. (II.44), (II.45) that



FIG. 2. The cross section for the initial states 2p, m=1 in spherical coordinates. Theoretically it should be equal to Q(2100).



FIG. 3. The cross section for the initial states 2s and 2p, m=0 in spherical coordinates. Theoretically the sum of these cross sections should be equal to Q(2010)+Q(2001).



FIG. 4. Ionization of the hydrogen in the n=2 level, averaged over all sublevels.



FIG. 5. Ionization of the hydrogen when the atom is in each of the sublevels of the level n=3.



F1G. 6. Ionization of the hydrogen in the n=3 level, averaged over all sublevels.

Then by Eq. (II.48) it follows that

$$S(n_1n_2|-k-K) = S(n_1n_2|kK).$$

Combining with the previous result, it follows that

 $S(n_2n_1|kK) = S(n_1n_2|k-K) = S(n_1n_2|-kK). \quad (II.49)$ 



FIG. 7. Ionization of the hydrogen in the n=4 level, averaged over all sublevels.

A case of particular interest is the ionization per unit energy range of the ejected electron at k=0; this corresponds to the excitation of the hydrogen atom to the state  $n \rightarrow \infty$ . Equation (II.47) shows that this cross section does not change with the interchange of  $n_1$  and  $n_2$ :



FIG. 8. Ionization of the hydrogen in the n=5 level, averaged over all sublevels.



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.

## Multiplicity of States and the Total Cross Section

Since  $n_1+n_2=n-m-1$ , the number  $n_1$  can take the values 0, 1, 2,  $\cdots$ , n-m-1, or n-m values. The same is true of  $n_2$ . Then the total number of combinations of



FIG. 10. Ionization cross section of the hydrogen in the n=1 level per unit velocity range of the ejected electron.  $v_1$  is the velocity of the electron before ejection, i.e., the averaged velocity of the electron in the ground state of the hydrogen atom.

 $n_1$  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

$$Q(nm) = (n-m)^{-1} \sum_{n=1}^{\infty} Q(nmn_1n_2).$$
 (II.51)



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.

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

$$Q(n) = (2n-1)^{-1} \sum_{m=0}^{n-1} \epsilon_m Q(nm), \qquad \text{(II.52)}$$

 $\epsilon_m$  defined in Eq. (II.10). Notice that the total number



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.

TABLE II. In this and the following tables and figures the cross section in parabolic coordinates is expressed as  $Q(nmn_1n_2)$ , with *n* the principal quantum number, *m* the absolute value of the magnetic quantum number, and  $n_1$ ,  $n_2$  the quantum numbers corresponding to coordinates  $\xi$ ,  $\eta$ . In this table the ionization of the 1s level is recalculated by the formula given by Massey and Mohr (Ref. 2) and is compared to Q(1000) as obtained from the general expression for ionization with an arbitrary initial state.

| Ry    | eV    | Q(1000) | Q(1s)   |
|-------|-------|---------|---------|
| 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 |

of states for a given n is

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

as it should be.

# III. RESULTS AND DISCUSSION

Using Eqs. (II.46)–(II.48), the ionization cross sections of all sublevels of hydrogen belonging to the principal quantum numbers n=1, 2, 3, 4, 5 have been calculated. The ionization cross section of one sublevel for each of the principal quantum numbers n=6, 7, 8, 9, 10 has also been computed. Since the ionization cross sections of all sublevels of any principal quantum number are approximately the same in parabolic coordinates, the latter calculation gives an indication of the ionization cross sections of n=6, 7, 8, 9, 10. Thus we have at our disposal the ionization cross sections of the first 10 levels of the hydrogen atom.

At the moment, aside from the Born approximation, the main calculation of ionization with applicability to higher states is the classical calculation. 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, there exists a maximum of this parameter beyond which ionization does not take place. An integration with respect to the impact parameter between zero and its maximum gives the ionization cross section. The result is

$$Q_i = (4/E_0)[n^2 - (1/E_0)],$$
 (III.1)

| Turnent      |             |             |         |       |                       | Q(2s)            |                |                | Q(2010) |              |
|--------------|-------------|-------------|---------|-------|-----------------------|------------------|----------------|----------------|---------|--------------|
| Impact<br>Rv | energy      | O(2h m = 1) | O(2100) | O(2s) | O(2 + m = 0)          | +<br>O(2, m = 0) | O(2010)        | O(2001)        | O(2001) | $\bar{Q}(2)$ |
| Ky           | C V         | Q(2p, m-1)  | Q(2100) | Q(23) | $Q(\mathbf{z}p, m=0)$ | Q(2p, m=0)       | 6(2010)        | 2(2001)        | £(1001) | ÷ (=)        |
| 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         |             | 17.48   |       |                       |                  | 17.14          | 17.14          | 20 50   | 17.31        |
| 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          | 30.02   | 17.84        |
| 1.44         | 19.6        | 14.14       | 14.20   | 13.31 | 17.34                 | 30.05            | 15.35          | 15.35          | 30.70   | 14.70        |
| 3.24         | 44.1        | 7.584       | 1.584   | 7.549 | 9.599                 | 17.148           | 8.373<br>5.703 | 8.374<br>5.702 | 11.149  | 5 320        |
| 5.29         | /1.9        | 4.950       | 4.950   | 5.079 | 0.320                 | 9 642            | 3.703          | 3.702          | 8 644   | 4 022        |
| 1.29         | 99.1<br>100 | 3.721       | 3.122   | 3.011 | 4.700                 | 0.045            | 4.322          | 4.522          | 0.011   | 4.022        |
|              | 200         | 1.061       |         | 2 110 | 2 520                 |                  |                |                |         |              |
|              | 300         | 1 348       |         | 1 475 | 1 744                 |                  |                |                |         |              |
|              | 400         | 1.031       |         | 1 156 | 1.352                 |                  |                |                |         |              |
|              | 500         | 0.838       |         | 0.950 | 1,103                 |                  |                |                |         |              |
|              | 600         | 0.707       |         | 0.810 | 0.934                 |                  |                |                |         |              |
|              | 700         | 0.612       |         | 0.707 | 0.812                 |                  |                |                |         |              |
|              | 800         | 0.541       |         | 0.629 | 0.719                 |                  |                |                |         |              |
|              | 900         | 0.484       |         | 0.567 | 0.647                 |                  |                |                |         |              |
|              | 1000        | 0.439       |         | 0.517 | 0.588                 |                  |                |                |         |              |
|              |             |             |         |       |                       |                  |                |                |         |              |

TABLE III. Ionization cross section in  $\pi a_0^2$  for the initial states 2s; 2p, m=0, 1 in spherical coordinates. The corresponding results in parabolic coordinates are also given and compared. The averaged ionization cross section for n=2 is designated by  $\bar{Q}(2)$ .

TABLE IV. The n=3 level ionization. The cross sections in  $\pi a_0^2$  due to all sublevels are listed for comparison. The averaged cross section is given in the last column.

| Impact | energy |         |         |         |         |         |         |            |
|--------|--------|---------|---------|---------|---------|---------|---------|------------|
| Ry     | eV     | Q(3200) | Q(3110) | Q(3101) | Q(3020) | Q(3002) | Q(3011) | $ar{Q}(3)$ |
| 0.11   | 1.5    | 0       | 0       | 0       | 0       | 0       | 0       | 0          |
| 0.16   | 2.2    | 60.1    | 56.2    | 56.2    | 50.8    | 51.1    | 56.9    | 56.0       |
| 0.22   | 3.0    | 91.5    | 93.0    | 92.8    | 89.4    | 89.0    | 93.6    | 91.8       |
| 0.36   | 4.9    | 91.3    | 99.5    | 99.3    | 101.3   | 100.8   | 99.5    | 98.0       |
| 0.64   | 8.7    | 66.0    | 75.4    | 75.2    | 80.1    | 80.0    | 75.2    | 74.3       |
| 1.0    | 13.6   | 46.4    | 54.1    | 54.1    | 55.9    | 59.1    | 49.3    | 52.6       |
| 4.0    | 54.4   | 13.3    | 15.8    | 15.8    | 17.5    | 14.1    | 13.6    | 15.0       |
|        |        |         |         |         |         |         |         |            |

TABLE V. The n=4 level ionization. The cross sections in  $\pi a_0^2$  due to all sublevels are listed for comparison. The averaged cross section is given in the last column.

| Energy              | impact             | 0(4300)          | 0(1210)          | 0(4201)          | 0(4120)           | 0(4102)           | 0(4111)          | 0(4020)           | 0(4002)           | 0(4021)          | 0(4012)          | ōw               |
|---------------------|--------------------|------------------|------------------|------------------|-------------------|-------------------|------------------|-------------------|-------------------|------------------|------------------|------------------|
| Ку                  | ev                 | Q(4300)          | Q(4210)          | Q(4201)          | Q(4120)           | Q(4102)           | Q(4111)          | Q(4030)           | Q(4003)           | Q(4021)          | Q(4012)          | Q(4)             |
| 0.0625              | 0.85               | 0                | 0                | 0                | 0                 | 0                 | 0                | 0                 | 0                 | 0                | 0                | 0                |
| 0.09                | 1.22               | 206              | 191              | 191              | 178               | 174               | 187              | 160               | 151               | 183              | 182              | 183              |
| 0.125               | 1.7                | 287              | 297              | 297              | 287               | 294               | 297              | 279               | 257               | 288              | 275              | 289              |
| 0.16                | 2.2                | 297              | 321              | 321              | 340               | 340               | 323              | 329               | 297               | 328              | 326              | 323              |
| 0.36                | 4.9                | 196              | 226              | 226              | 249               | 248               | 232              | 250               | 221               | 228              | 212              | 229              |
| 0.64                | 8.7                | 121              | 138              | 143              | 155               | 162               | 147              | 171               | 145               | 145              | 135              | 146              |
| 1.0                 | 13.6               | 81               | 92               | 96               | 105               | 111               | 87               | 119               | 100               | 93               | 92               | 97               |
| 0.36<br>0.64<br>1.0 | 4.9<br>8.7<br>13.6 | 196<br>121<br>81 | 226<br>138<br>92 | 226<br>143<br>96 | 249<br>155<br>105 | 248<br>162<br>111 | 232<br>147<br>87 | 250<br>171<br>119 | 221<br>145<br>100 | 228<br>145<br>93 | 212<br>135<br>92 | 229<br>146<br>97 |

TABLE VI. The n=5 level ionization. The cross section in  $\pi a_0^2$  due to all sublevels are listed for comparison. The averaged cross section is given in the last column.

| Impact                                                | energy                                            |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                            |                                             |                                             |                                             |                                             |
|-------------------------------------------------------|---------------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|--------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|
| Ry                                                    | 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(5004)                                     | $\overline{Q}(5)$                           |
| 0.04<br>0.0625<br>0.09<br>0.16<br>0.36<br>0.64<br>1.0 | 0.54<br>0.85<br>1.22<br>2.2<br>4.9<br>8.7<br>13.6 | 0<br>586<br>724<br>593<br>321<br>185<br>120 | 0<br>569<br>775<br>695<br>358<br>218<br>144 | 0<br>569<br>777<br>670<br>365<br>218<br>144 | 0<br>539<br>791<br>758<br>408<br>245<br>166 | 0<br>543<br>806<br>759<br>408<br>250<br>166 | 0<br>558<br>784<br>722<br>388<br>213<br>139 | 0<br>505<br>784<br>800<br>448<br>275<br>180 | 0<br>505<br>784<br>797<br>420<br>256<br>149 | 0<br>539<br>740<br>743<br>387<br>222<br>146 | 0<br>539<br>784<br>740<br>375<br>200<br>132 | 0<br>472<br>754<br>796<br>470<br>286<br>193 | 0<br>435<br>668<br>671<br>318<br>139<br>96 | 0<br>515<br>774<br>753<br>412<br>240<br>159 | 0<br>481<br>704<br>668<br>340<br>186<br>124 | 0<br>515<br>734<br>683<br>362<br>211<br>139 | 0<br>533<br>765<br>725<br>386<br>225<br>147 |
|                                                       |                                                   |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                             |                                            |                                             |                                             |                                             |                                             |

TABLE VII. The cross section for ionization from the levels n=6, 7, 8, 9, 10 in units of  $\pi a_0^2$ . 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.

| Ry     | eV   | Q(6500) | Q(7600) | Q(8700) | Q(9800) | Q(10 900) |
|--------|------|---------|---------|---------|---------|-----------|
| 0.0121 | 0.16 |         |         |         |         | 4935      |
| 0.0144 | 0.20 |         |         |         | 2514    | 8550      |
| 0.0225 | 0.31 |         |         | 3441    | 7137    | 11096     |
| 0.0256 | 0.35 |         | 1307    | 4140    | 7350    | 10742     |
| 0.0400 | 0.54 | 1056    | 2697    | 4498    | 6408    | 8449      |
| 0.0900 | 1.22 | 1339    | 2009    | 2761    | 3608    | 4542      |
| 0.1600 | 2.2  | 921     | 1292    | 1705    | 2154    | 2642      |
| 0.3600 | 4.9  | 448     | 608     | 788     | 990     | 1212      |
| 0.6400 | 8.7  | 262     | 341     | 437     | 564     | 687       |
| 1.0000 | 13.6 | 170     | 227     | 290     | 362     | 440       |

where  $Q_i$  is the cross section in units of  $\pi a_0^2$ ,  $E_0$  is the impact energy in rydbergs, 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 quantum-mechanical Born calculation, although it gives a smaller cross section and the position of the maximum is displaced. An improvement in Thomson's calculation is to take the motion of the bound electron into account. This has been done approximately by Gryzinski.<sup>23</sup> Let us introduce  $a = (n^2 E_0)^{-1}$ ; then according to this author Eq. (III.1) should be replaced by

$$Q_i = \sigma_0 n^4 g(n, E_0), \qquad (\text{III.2})$$

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

$$g(n, E_0) = a(1+a)^{-3/2} \times \begin{cases} [(5/3) - 2a]], & a \le \frac{1}{2} \\ (4\sqrt{2}/3)(1-a)^{3/2}, & a \ge \frac{1}{2}. \end{cases}$$
(III.3)

It should be noticed that in both Eqs. (III.1) and (III.2) the cross section falls off asymptotically as  $E_0^{-1}$ . while in a quantum-mechanical Born calculation the corresponding asymptotic form is  $\ln E_0/E_{0.24}$ 

For comparison, in Fig. 1 the Born, the classical, and the 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.

In Tables I-VIII and in Figs. 2-14, the total and the partial ionization cross sections are recorded and displayed. For n=1 and 2, in addition to parabolic coordinates, spherical coordinates have been used, and the calculated values are recorded and compared.

Let the wave functions in parabolic and spherical coordinates be represented by  $\psi(nmn_1n_2)$  and  $\phi(nlm)$ , then for n=2,

$$\psi(2010) = (1/\sqrt{2}) [\phi(2s) + \phi(2p0)] 
\psi(2001) = (1/\sqrt{2}) [\phi(2s) - \phi(2p0)],$$
(III.4)

and by Eqs. (II 2), (II 5),

$$Q(2010) + Q(2001) = Q(2s) + Q(2p0)$$
, (III.5)

The above equivalence is indicated in Table III and Fig. 3.

Originally the ionization of the 2s and the 2p, m=0states was computed numerically by Swan.<sup>6</sup> Swan's results are larger approximately by a factor of 2 because of being incorrectly multiplied by a factor of 2 and being obtained by a cruder method of numerical integration.<sup>25</sup>

A study of the figures and tables indicates the following observations:

(1) The ionization cross section of excited states grows as fast as the classical law of  $n^4 \pi a_0^2$  only for incident energies large compared with the ionization energy of the level concerned. For intermediate energies the cross section grows less rapidly.

(2) Most of the contribution to the cross section is from the region of zero-energy ejected electrons, k=0, as is seen from Table VIII. At k=0, the interchange of  $n_1$  and  $n_2$  does not change the partial cross section [cf. Eq. (II 50)]. Figure 5 shows that, because of the large contribution of the k=0 region, when  $n_1$  and  $n_2$  are interchanged the total cross section remains the same to about three significant figures.<sup>26</sup> The k=0 region contribution is consistent with the assumption made about the wave functions of the two electrons.

(3) The ionization cross sections of different sublevels in a given level are comparable to each other in parabolic coordinates.

(4) The maxima of partial cross sections in Figs. 10-14 occur when the velocity of the ejected electron is half its velocity before ejection. The repetition of this pattern for ionization of n=1, 2, 3, 4, 5, averaged over all substates, is in agreement with the classical theory of ionization in which the excited-state cross sections can be obtained from the ground-state cross section by appropriate scaling of energies of the incident and the ejected electrons. However, the fact that remains unexplained is that the maxima have the same positions for all values of the incident energies.

In all the tables the last significant figure may be in error by a few units. In a few cases, especially for higher values of n, the next-to-the-last significant figure may also be in error by a few units.

In a calculation which will be reported later, extension of the present theory to the higher excited states of hydrogen will be considered.

<sup>23</sup> M. Gryzinski, Phys. Rev. 115, 374 (1958); 138, A305 (1965). An improvement upon the calculation of Gryzinski is performed by R. C. Stabler [Phys. Rev. 133, A1268 (1964)] in which a subsidiary approximation made by Gryzinski in averaging the cross section over the initial angular distribution of the bound electron is dropped. The result, however, is in less agreement with the experiment. Here we quote only Gryzinski's results. <sup>24</sup> See Ref. 16, Eq. (20.5).

<sup>&</sup>lt;sup>25</sup> T. J. M. Boyd, Proc. Phys. Soc. (London) 72, 523 (1958), and D. McCrea and T. V. M. McKirgan, *ibid.* 75, 235 (1960), in de-termination of the ionization of the 2s and 2p, m=0 states with zero velocity ejected electrons, find similar discrepancies.

<sup>&</sup>lt;sup>26</sup> The asymmetry in the cross sections, which apparently causes the weakening of some Stark components in a canal ray tube, is due to the higher order corrections in the cross section. See E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra (Cam-bridge University Press, New York, 1963), Chap. 17, Sec. 1.

|                                                                                   |                                                                                   |                                                                                   |                                                                                  |                                                                              | (a) $n = 1$                                                                                           | l                                                                         |                                                     |                               |                    |         |
|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|----------------------------------------------------------------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------|-----------------------------------------------------|-------------------------------|--------------------|---------|
| $k_0^2$                                                                           | 0                                                                                 | 1/256                                                                             | 1/64                                                                             | 1/16                                                                         | 1/4                                                                                                   | 9/16                                                                      | 1                                                   | 9/4                           | 4                  | 25/4    |
| $1.0 \\ 1.44 \\ 1.96 \\ 2.00 \\ 2.56 \\ 3.24 \\ 4.00 \\ 6.25 \\ 9.00$             | 0<br>2.6148<br>2.7376<br>2.7304<br>2.5614<br>2.3216<br>2.0844<br>1.5942<br>1.2473 | 0<br>2.5828<br>2.7085<br>2.7014<br>2.5350<br>2.2976<br>2.0627<br>1.5772<br>1.2337 | 2.4881<br>2.6235<br>2.6169<br>2.4578<br>2.2277<br>1.9995<br>1.5277<br>1.1941     | 2.1419<br>2.3166<br>2.3121<br>2.1796<br>1.9763<br>1.7724<br>1.3502<br>1.0525 | $\begin{array}{c} 1.1175\\ 1.4642\\ 1.4667\\ 1.4150\\ 1.2886\\ 1.1537\\ 0.87048\\ 0.67209\end{array}$ | 0.72071<br>0.73398<br>0.77583<br>0.72091<br>0.64715<br>0.48371<br>0.36901 | 0.37420<br>0.37786<br>0.34517<br>0.25764<br>0.19443 | 0.09409<br>0.07860<br>0.05890 | 0.02710<br>0.02160 | 0.00903 |
|                                                                                   |                                                                                   |                                                                                   |                                                                                  |                                                                              | (b) $n = 2$                                                                                           | 2                                                                         |                                                     |                               |                    |         |
| $k_0^2$                                                                           | 0                                                                                 | 1/256                                                                             | 1/64                                                                             | 1/16                                                                         | 1/4                                                                                                   | 9/16                                                                      | 1                                                   | 9/4                           | 1                  | 25/4    |
| 0.25<br>0.36<br>0.50<br>0.64<br>1.00<br>1.44<br>3.24<br>5.29<br>7.29              | 0<br>185.6<br>181.3<br>163.1<br>124.6<br>96.20<br>51.07<br>34.10<br>26.04         | 0<br>176.7<br>174.0<br>156.7<br>119.7<br>92.34<br>48.93<br>32.63<br>24.91         | 0<br>153.0<br>154.4<br>139.5<br>106.5<br>82.00<br>43.21<br>28.73<br>21.89        | 0<br>81.58<br>99.48<br>91.87<br>70.32<br>53.80<br>27.83<br>18.31<br>13.86    | 25.55<br>21.95<br>16.73<br>8.317<br>5.334<br>3.972                                                    | 6.283<br>5.296<br>2.602<br>1.640<br>1.208                                 | 1.768<br>0.9803<br>0.6131<br>0.4491                 | 0.2147<br>0.1361<br>0.0994    | 0.0443<br>0.0326   | 0.0133  |
|                                                                                   |                                                                                   |                                                                                   |                                                                                  |                                                                              | (c) $n = 3$                                                                                           | 3                                                                         |                                                     |                               |                    |         |
| $k_0^2$                                                                           | 0                                                                                 | 1/256                                                                             | 1/64                                                                             | 1/16                                                                         | 1/4                                                                                                   | 9/16                                                                      | 1                                                   | 9/4                           |                    |         |
| $\begin{array}{c} 0.11\\ 0.16\\ 0.22\\ 0.36\\ 0.64\\ 1.00\\ 4.00\\ \end{array}$   | $0\\224+1\\215+1\\164+1\\107+1\\740\\227$                                         | 0<br>201+1<br>196+1<br>150+1<br>977<br>672<br>204                                 | $0\\144+1\\137+1\\118+1\\761\\522\\154$                                          | 610<br>535<br>346<br>235<br>65.0                                             | 61.0<br>40.3<br>10.0                                                                                  | 9.51<br>2.27                                                              | 0.704                                               | 0.099                         |                    |         |
|                                                                                   |                                                                                   |                                                                                   |                                                                                  |                                                                              | (d) $n = -$                                                                                           | 4                                                                         |                                                     |                               |                    |         |
| $k_0^2$                                                                           | 0                                                                                 | 1/256                                                                             | 1/64                                                                             | 1/16                                                                         | 1/4                                                                                                   | 9/16                                                                      |                                                     |                               |                    |         |
| 0.0625<br>0.09<br>0.125<br>0.16<br>0.36<br>0.64<br>1.00                           | $0 \\ 130+2 \\ 124+2 \\ 109+2 \\ 595+1 \\ 366+1 \\ 248+1$                         | $0\\106+2\\105+2\\934+1\\506+1\\311+1\\210+1$                                     | $\begin{array}{r} 0\\ 549+1\\ 676+1\\ 616+1\\ 334+1\\ 203+1\\ 136+1 \end{array}$ | 169+1<br>105+1<br>628<br>407                                                 | 102<br>68.2<br>42.1                                                                                   | 7.75<br>7.94                                                              |                                                     |                               |                    |         |
|                                                                                   |                                                                                   |                                                                                   |                                                                                  |                                                                              | (e) $n = 5$                                                                                           |                                                                           |                                                     |                               |                    |         |
| $k_0^2$                                                                           | 0                                                                                 | 1/256                                                                             | 1/64                                                                             | 1/16                                                                         | 1/4                                                                                                   | 9/16                                                                      |                                                     |                               |                    |         |
| $\begin{array}{c} 0.04\\ 0.0625\\ 0.09\\ 0.16\\ 0.36\\ 0.64\\ 1.00\\ \end{array}$ | 0498+2461+2315+2158+2942+1630+1                                                   | $0 \\ 372+2 \\ 358+2 \\ 247+2 \\ 122+2 \\ 709+1 \\ 471+1$                         | $0 \\ 139+2 \\ 189+2 \\ 136+2 \\ 650+1 \\ 371+1 \\ 244+1 $                       | 298+1<br>141+1<br>794<br>505                                                 | 105<br>60.9<br>38.2                                                                                   | 6.82<br>5.12                                                              |                                                     |                               |                    |         |

TABLE VIII. The ionization cross section per unit energy range of the ejected electron for the first five levels of hydrogen.  $k_0^2$  and  $k^2$  are the energies of the incident and ejected electrons in rydbergs. The cross section for a given  $k_0^2$  and  $k^2$  has been averaged over all sublevels for the particular level concerned. 224+1 means  $224\times10^{+1}$ , etc.

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