Excitation by Electron Collision of Excited Atomic Hydrogen

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The atomic form factor of the hydrogen atom with arbitrary initial and final states is evaluated in closed form using parabolic coordinates. Using this expression the cross section for excitation of the hydrogen atom by electron collision in the Born approximation is evaluated. The total cross sections in the energy range of interest for transitions between the following principal quantum numbers are tabulated: $n=1$ to $n'=2, 3, 4, 5, 6, 7, 8, 9, 10$; $n=2$ to $n'=3, 4, 5, 6, 7, 8$; $n=3$ to $n'=4, 5, 6, 7, 8$; $n=4$ to $n'=5, 6$; $n=5$ to $n'=6$. In conclusion, a curve for the total of inelastic collisions of electrons with the hydrogen atom in its first five energy levels is constructed. The expression for the atomic form factor may be used in the evaluation of the generalized oscillator strength and in the calculation of the dispersion of x rays in atoms.

I. INTRODUCTION

THE excitation cross section in hydrogen induced by electron collision, calculated in the Born approximation, is proportional to the squared modulus of the atomic form factor given by

$$V(i,f)=\int e^{iKz}\psi_i^*(\mathbf{r})\psi_f(\mathbf{r})d^3r,$$

where ψ_i and ψ_f are the initial and final eigenfunctions of the atomic electron and K is the magnitude of momentum transfer of the incident electron. In this paper a closed form is found for the above expression when ψ_i and ψ_f are hydrogenic functions expressed in parabolic coordinates. Elwert[1] has evaluated this expression with similar specifications, although his final result is in differential form.

The main concern of this paper is the evaluation of the cross section for electron-impact-induced excitation between two arbitrary levels of hydrogen, calculated in the Born approximation. Up to now many such calculations in the Born approximation have been carried out, and tables of cross sections with initial states in the range of principal quantum numbers 1–5 and final states with principal quantum numbers 2–10 are available,[2–10] although for higher levels the calculations are only for certain substates.

In this paper, before tabulation, the results in parabolic coordinates are compared with those in spherical coordinates, and their consistency is examined. The calculation is then extended to higher levels, for which results in spherical coordinates are not available. All cross sections are listed in tables. It is hoped that these tables will be useful in plasma and astrophysical calculations.

II. FORMULATION

Excitation Amplitude

Let the propagation vector of the exciting electron before and after collision be designated by $\mathbf{k}_0$ and $\mathbf{k}_1$, and the states of the atom in parabolic coordinates before and after collision by n_1n_2m and $n_1'n_2'm'$. The excitation cross section in atomic units for such a collision is then given by[11]

$$Q(n_1n_2m,n_1'n_2'm')=\frac{8\pi}{k_0^2}\int_{k_0-k_1}^{k_0+k_1}|V(n_1n_2m,n_1'n_2'm')|^2\frac{dK}{K^3},\tag{1}$$

$$\begin{aligned}V(n_1n_2m,n_1'n_2'm')&=\int e^{iKz}\phi^*_{n_1n_2m}(\xi\eta\phi)\phi_{n_1'n_2'm'}(\xi\eta\phi)\tfrac{1}{4}(\xi+\eta)d\xi d\eta d\phi\\&=\delta(m,m')\tfrac{1}{4}N_{n_1n_2}N_{n_1'n_2'}\int_0^\infty\int_0^\infty\exp\left[\frac{iK}{2}(\xi-\eta)-\tfrac{1}{2}(\alpha+\alpha')(\xi+\eta)\right]\\&\quad\times(\xi\eta)^mL_{n_1+m}{}^m(\alpha\xi)L_{n_1'+m}{}^m(\alpha'\xi)L_{n_2+m}{}^m(\alpha\eta)L_{n_2'+m}{}^m(\alpha'\eta)(\xi+\eta)d\xi d\eta.\end{aligned}\tag{2}$$

[1] G. Elwert, Z. Naturforsch. **10a**, 361 (1955).
[2] L. Goldstein, Ann. Physik **19**, 305 (1933).
[3] B. M. Yavorsky, Compt. Rend. Acad. Sci. U.R.S.S. **43**, 151 (1944).
[4] R. McCarroll, Proc. Phys. Soc. (London) **A70**, 460 (1957). Cross section for the transitions $nl=1s\rightarrow n'=2, 3, 4, 5, 6$.
[5] T. J. M. Boyd, Proc. Phys. Soc. (London) **72**, 523 (1958). Cross section for the transitions $nl=2s\rightarrow n'=3, 4, 5, 6, 7, 8, 9, 10$.
[6] D. McCrea and T. V. M. McKirgan, Proc. Phys. Soc. (London) **75**, 235 (1960). Cross section for the transitions $nlm=2p0, \pm1\rightarrow n'=3, 4, 5, 6, 7, 8, 9, 10$.
[7] G. C. McCoyd, S. N. Milford, and J. J. Wahl, Phys. Rev. **119**, 149 (1960). Cross section for the transitions $n=3\rightarrow n'=4$ and $3s\rightarrow 5p$, $3p\rightarrow 5d$, $3d\rightarrow 5f$.
[8] L. Fisher, S. N. Milford, and F. R. Pomilla, Phys. Rev. **119**, 153 (1960). Cross section for the transitions $4s\rightarrow 5p$, $4p\rightarrow 5d$, $4d\rightarrow 5f$, $4f\rightarrow 5g$, $4s\rightarrow 6p$, $4f\rightarrow 6g$.
[9] S. N. Milford, J. J. Morrissey, and J. H. Scanlon, Phys. Rev. **120**, 1715 (1960). Cross section for the transitions $5s\rightarrow 6p$, $5p\rightarrow 6d$, $5d\rightarrow 6f$, $5f\rightarrow 6g$, $5g\rightarrow 6h$. See also J. H. Scanlon and S. N. Milford, Astron. J. **134**, 724 (1961).
[10] G. C. McCoyd and S. N. Milford, Phys. Rev. **130**, 206 (1963). Cross section for the transitions $10s\rightarrow 11p$ and $n=10$, $l=9\rightarrow n'=11$, $l'=10$.
[11] K. Omidvar, Phys. Rev. **140**, A26 (1965), Eqs. (II.4). This report precedes the present paper and will be designated from now on as I.

$N_{n_1n_2}$ is the normalization factor of the ξ, η eigenfunctions given in I; similarly, $N_{n_1'n_2'}$ is the factor corresponding to ξ', η'. With this equation and the generating function of the associated Laguerre functions it follows that

$$\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_1'=0}^{\infty}\sum_{n_2'=0}^{\infty}\frac{s^{n_1}s'^{n_1'}t^{n_2}t'^{n_2'}}{(n_1+m)!(n_1'+m)!(n_2+m)!(n_2'+m)!}V(n_1n_2m,n_1'n_2'm)$$

$$=\frac{\frac{1}{4}N_{n_1n_2}N_{n_1'n_2'}}{[(1-s)(1-t)(1-s')(1-t')]^{m+1}}\int_0^\infty\int_0^\infty\exp\left[\frac{iK}{2}(\xi-\eta)-\tfrac{1}{2}(\alpha+\alpha')(\xi+\eta)\right]$$

$$\times\exp\left[-\left(\frac{\alpha s}{1-s}+\frac{\alpha's'}{1-s'}\right)\xi-\left(\frac{\alpha t}{1-t}+\frac{\alpha't'}{1-t'}\right)\eta\right]\times(\xi\eta)^m(\xi+\eta)d\xi d\eta$$

$$=\frac{-\frac{1}{4}N_{n_1n_2}N_{n_1'n_2'}}{[(1-s)(1-t)(1-s')(1-t')]^{m+1}}\frac{\partial U}{\partial p}, \tag{3}$$

where we have introduced

$$p=\tfrac{1}{2}(\alpha+\alpha'),\quad q=-iK/2, \tag{4}$$

$$U=\int_0^\infty\exp\left[-\left(p+q+\frac{\alpha s}{1-s}+\frac{\alpha's'}{1-s'}\right)\xi\right]\xi^m d\xi\int_0^\infty\exp\left[-\left(p-q+\frac{\alpha t}{1-t}+\frac{\alpha't'}{1-t'}\right)\eta\right]\eta^m d\eta$$

$$=(m!)^2\left(p+q+\frac{\alpha s}{1-s}+\frac{\alpha's'}{1-s'}\right)^{-(m+1)}\left(p-q+\frac{\alpha t}{1-t}+\frac{\alpha't'}{1-t'}\right)^{-(m+1)}. \tag{5}$$

By means of a Taylor's expansion we obtain[12]

$$\left(p+q+\frac{\alpha s}{1-s}+\frac{\alpha's'}{1-s'}\right)^{-(m+1)}=\sum_{l_1l_1'\nu_1\nu_1'}(l_1!l_1'!)^{-1}(-)^{\nu_1+\nu_1'}\times\frac{(m+\nu_1+\nu_1')!}{m!}$$

$$\times C(\nu_1l_1)C(\nu_1'l_1')\alpha^{\nu_1}\alpha'^{\nu_1'}\times a^{-(m+1+\nu_1+\nu_1')}\times s^{l_1}s'^{l_1'}, \tag{6}$$

where we have introduced

$$a=p+q=\tfrac{1}{2}(\alpha+\alpha'-iK). \tag{7}$$

The coefficients $C(\nu l)$ are defined in I. Similarly,

$$\left(p-q+\frac{\alpha t}{1-t}+\frac{\alpha't'}{1-t'}\right)^{-(m+1)}=\sum_{l_2l_2'\nu_2\nu_2'}(l_2!l_2'!)^{-1}(-)^{\nu_2+\nu_2'}\times\frac{(m+\nu_2+\nu_2')!}{m!}$$

$$\times C(\nu_2l_2)C(\nu_2'l_2')\alpha^{\nu_2}\alpha'^{\nu_2'}a^{*-(m+1+\nu_1+\nu_1')}t^{l_2}t'^{l_2'}. \tag{8}$$

When these equations are substituted in Eq. (5) and note is taken of the relation

$$\frac{\partial U}{\partial p}=\left(\frac{\partial}{\partial a}+\frac{\partial}{\partial a^*}\right)U, \tag{9}$$

the right-hand side of Eq. (3) becomes, after making a binomial expansion of its denominator,

$$\tfrac{1}{4}N_{n_1n_2}N_{n_1'n_2'}\sum_{j_1j_1'j_2j_2'}\sum_{l_1l_1'\nu_1\nu_1'l_2l_2'\nu_2\nu_2'}\binom{m+j_1}{j_1}\binom{m+j_1'}{j_1'}\binom{m+j_2}{j_2}\binom{m+j_2'}{j_2'}(l_1!l_1'!l_2!l_2'!)^{-1}(-)^{\nu_1+\nu_1'+\nu_2+\nu_2'}$$

$$\times(m+\nu_1+\nu_1')!(m+\nu_2+\nu_2')!C(\nu_1l_1)C(\nu_1'l_1')C(\nu_2l_2)C(\nu_2'l_2')\alpha^{\nu_1+\nu_2}\alpha'^{\nu_1'+\nu_2'}a^{-(m+2+\nu_1+\nu_1')}a^{*-(m+2+\nu_2+\nu_2')}$$

$$\times[(m+1+\nu_1+\nu_1')a^*+(m+1+\nu_2+\nu_2')a]s^{j_1+l_1}s'^{j_1'+l_1'}t^{j_2+l_2}t'^{j_2'+l_2'}.$$

Equating the coefficients of equal powers of s, s', t, t' of this equation and the left-hand side of Eq. (3), substituting the value

$$N_{n_1n_2}=\left(\frac{2}{n}\right)^{1/2}\alpha^{m+3/2}\left[\frac{n_1!n_2!}{(n_1+m)!^3(n_2+m)!^3}\right]^{1/2},\quad\alpha=\frac{Z}{n}, \tag{10}$$

[12] For details of expansion see K. Omidvar, External Report X-641-64-193, Goddard Space Flight Center, Greenbelt, Maryland (unpublished).

and making use of Eq. (7), we obtain

$$V(n_1n_2m,n_1'n_2'm)=A\sum_{\gamma=1}^{N}G(\gamma)H(\gamma)\,, \tag{11}$$

where

$$A=\tfrac{1}{2}(2Z)^{2m+3}(nn')^{-(m+2)}\times\left[\frac{n_1!n_2!n_1'!n_2'!}{(n_1+m)!(n_2+m)!(n_1'+m)!(n_2'+m)!}\right]^{1/2}, \tag{12}$$

$$G(\gamma)=(-2)^{\nu_1+\nu_2+\nu_1'+\nu_2'}\binom{m+j_1}{j_1}\binom{m+j_2}{j_2}\binom{m+j_1'}{j_1'}\binom{m+j_2'}{j_2'}(l_1!l_2!l_1'!l_2'!)^{-1}(m+\nu_1+\nu_1')!(m+\nu_2+\nu_2')!$$
$$\times C(\nu_1l_1)C(\nu_2l_2)C(\nu_1'l_1')C(\nu_2'l_2')\alpha^{\nu_1+\nu_2}\alpha'^{\nu_1'+\nu_2'}, \tag{13}$$

$$H(\gamma)=(\alpha+\alpha'-iK)^{-(m+2+\nu_1+\nu_1')}\times(\alpha+\alpha'+iK)^{-(m+2+\nu_2+\nu_2')}$$
$$\times[(2m+2+\nu_1+\nu_2+\nu_1'+\nu_2')(\alpha+\alpha')+i(\nu_1+\nu_1'-\nu_2-\nu_2')K]. \tag{14}$$

γ stands for the set of 12 variable integers,

$$\gamma=(j_1j_2j_1'j_2'l_1\nu_1l_2\nu_2l_1'\nu_1'l_2'\nu_2')\,, \tag{15}$$

subject to the restrictions

$$\begin{aligned}
&l_1=0,1,2,\cdots,n_1; \quad j_1=n_1-l_1; \quad \nu_1=0,1,2,\cdots,l_1;\\
&l_2=0,1,2,\cdots,n_2; \quad j_2=n_2-l_2; \quad \nu_2=0,1,2,\cdots,l_2;\\
&l_1'=0,1,2,\cdots,n_1'; \quad j_1'=n_1'-l_1'; \quad \nu_1'=0,1,2,\cdots,l_1';\\
&l_2'=0,1,2,\cdots,n_2'; \quad j_2'=n_2'-l_2'; \quad \nu_2'=0,1,2,\cdots,l_2';
\end{aligned} \tag{16}$$

and N is the total number of combinations of the 12 integers for a given $n_1n_2n_1'n_2'$.

Substitution of Eq. (11) in Eq. (1) and a numerical integration with respect to K allows the cross section between two arbitrary states to be determined. When N is not very large, it is advantageous to carry out the integration with respect to K analytically. Through Eqs. (1), (11) we can write

$$Q(n_1n_2m,n_1'n_2'm)=\frac{8\pi A^2}{k_0^2}\sum_{\gamma_1=1}^{N}\sum_{\gamma_2=1}^{N}G(\gamma_1)G(\gamma_2)$$
$$\times\int_{K_1}^{K_2}H(\gamma_1)H^*(\gamma_2)\frac{dK}{K^3}. \tag{17}$$

With the form of $H(\gamma)$ given in Eq. (14), the integration with respect to K is straightforward.

Symmetry Considerations

It is evident from Eq. (2) that

$$V(n_1n_2m,\,n_1'n_2'm|-K)=V^*(n_1n_2m,n_1'n_2'm|K)\,,$$
$$V(n_2n_1m,\,n_2'n_1'm|-K)=V(n_1n_2m,n_1'n_2'm|K)\,.$$

It follows that

$$|V(n_1n_2m,\,n_1'n_2'm|-K)|^2=|V(n_2n_1m,n_2'n_1'm|K)|^2$$
$$=|V(n_1n_2m,n_1'n_2'm|K)|^2; \tag{18}$$

and, by Eq. (1)

$$Q(n_2n_1m,n_2'n_1'm)=Q(n_1n_2m,n_1'n_2'm)\,. \tag{19}$$

The cross section for an initial state n_1n_2m and a final state $n'm$ is obtained by summing the above equation over $n_1'n_2'$. We obtain in this way

$$Q(n_2n_1m,n'm)=Q(n_1n_2m,n'm)\,. \tag{20}$$

Similarly by averaging the initial states over n_1n_2 we obtain

$$Q(nm,n_2'n_1'm)=Q(nm,n_1'n_2'm)\,. \tag{21}$$

For a given nm, the state n_2n_1 is the reflection of the n_1n_2 state with respect to the $z=0$ plane. For $n_1>n_2$ most of the electronic charge lies on the positive z axis, and for $n_1<n_2$ it lies on the negative z axis. Equations (20) and (21) indicate that the initial or the final states that are the mirror images of each other with respect to the $z=0$ plane have equal excitation cross sections.[13]

Equations (18), (19) are used to test the accuracy of the numerical results.

Multiplicity of States and the Total Cross Section

Since the direction of the z axis is taken along the momentum transfer vector **K**, the magnetic quantum number does not change in any transition. As $n_1+n_2=n-m-1$, 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 n_1 and n_2 for a given n and

[13] The asymmetry in the cross sections which apparently is the cause of the weakening of some components of Stark lines in a canal ray tube is due to higher order corrections in the cross sections. See E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, New York, 1963), Chap. 17, Sec. 1.

m is $n-m$. Similarly, the total number of combinations of n_1' and n_2' for a given n' and m' is $n'-m'$.

Designating the cross section for the transition $nn_1n_2m \rightarrow n'n_1'n_2'm$ by $Q(nn_1n_2m,n'n_1'n_2'm)$, the cross section for the transition $nn_1n_2m \rightarrow n'm$ is obtained by summing the former cross section over all the final states with a fixed m,

$$Q(nn_1n_2m,n'm)=\sum_{n_1'=0}^{n'-m-1} Q(nn_1n_2m,n'n_1'n_2'm). \quad (22)$$

The cross section for the transition $nm \rightarrow n'm$ is obtained by averaging $Q(nn_1n_2m,n'm)$ over all the initial states with a fixed m,

$$Q(nm,n'm)=(n-m)^{-1}\sum_{n_1=0}^{n-m-1} Q(nn_1n_2m,n'm). \quad (23)$$

The cross section for the transition $n \rightarrow n'$ is obtained by averaging $Q(nm,n'm)$ with respect to the magnitude of the magnetic quantum number m,

$$Q(n,n')=(2n-1)^{-1}\sum_{m=0}^{n-1}[2-\delta(m,0)]Q(nm,n'm). \quad (24)$$

Since the total number of the initial states is

$$\sum_{m=0}^{n-1}[2-\delta(m,0)](n-m)=n^2, \quad (25)$$

Eq. (24) can be written alternatively as

$$Q(n,n')=n^{-2}\sum_{m=0}^{n-1}\sum_{n_1=0}^{n-m-1}[2-\delta(m,0)] \times Q(nn_1n_2m,n'm). \quad (26)$$

It is interesting to note that the total number of independent transitions between the levels n and n' is given by

$$N=\sum_{m=0}^{n-1}[2-\delta(m,0)](n-m)(n'-m).$$

When the right-hand side is evaluated we obtain

$$N=n^2[n'-(n/3)]+(n/3). \quad (27)$$

III. RESULTS AND DISCUSSION

The excitation cross sections of the hydrogen atom by electron collision have been calculated for the transitions $n=1$ to $n'=2, 3, 4, 5, 6, 7, 8, 9, 10$; $n=2$ to $n'=3, 4, 5, 6, 7, 8$; $n=3$ to $n'=4, 5, 6, 7, 8$; $n=4$ to $n'=5, 6$; and $n=5$ to $n'=6$ in Born approximation and parabolic coordinates. Similar calculations in the Born approximation using sperhical coordinates have previously been made by McCarroll[4]; Boyd[5]; McCrea and McKirgan[6]; and McCoyd, Milford, and Wahl.[7–10] There are a few other calculations for certain optically allowed transitions between sublevels of higher levels, but they do not give the total transition cross section between two levels.

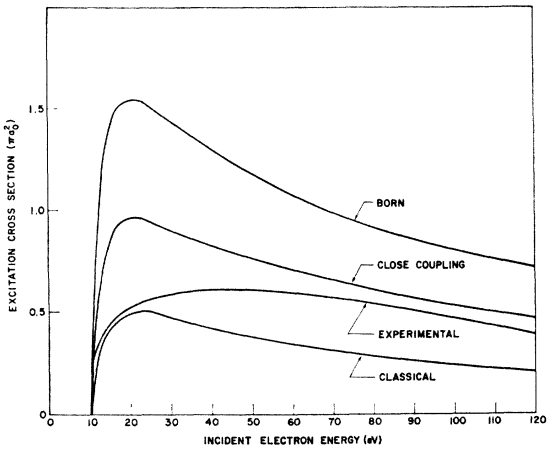

FIG. 1. Excitation of the ground state of the hydrogen atom to the $n=2$ states by electron collision. The theoretical curves—Born, close coupling, and classical—are compared with the experimental curve.

The excitation cross sections obtained in parabolic coordinates were compared to those previously obtained in spherical coordinates and their agreements were verified.[14] Since the set of wave functions due to a principal quantum number n in one coordinate system is given as linear combinations of the set of wave functions in the other coordinate system, the sum of

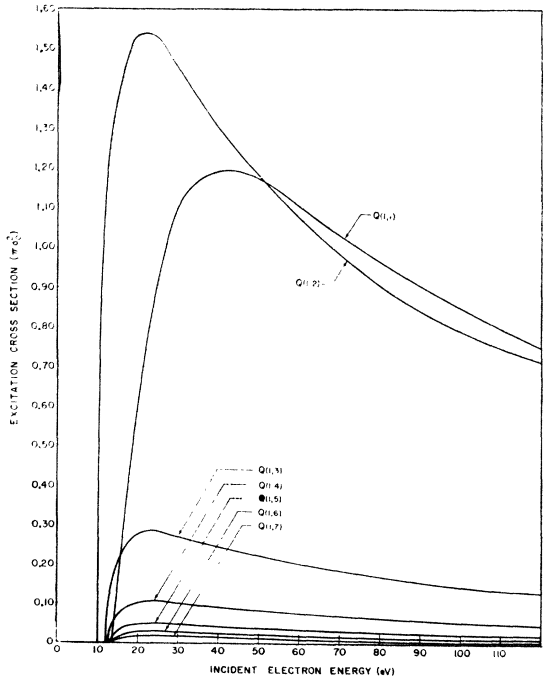

FIG. 2. Excitation of the ground state of the hydrogen to the $n=2, 3, 4, 5, 6, 7$ states. $Q(1,i)$ is the cross section of the ground state for ionization by electron collision.

[14] See Ref. 12.

TABLE I. Excitation cross sections of $n=1$ level in units of πa_0^2.

Impact energy Ry	eV	$Q(1,2)$	$Q(1,3)$	$Q(1,4)$	$Q(1,5)$	$Q(1,6)$	$Q(1,7)$	$Q(1,8)$	$Q(1,9)$	$Q(1,10)$	$\sum_{m=n+1}^{\infty} Q(1,m)$	$Q(T)$
1.00	13.60	1.2868	0.1787	0.0509	0.0199	0.0092	0.0050	0.0032	0.0018	0.0012	0.0016	1.5583
1.44	19.58	1.5354	0.2782	0.1000	0.0476	0.0265	0.0163	0.0104	0.0075	0.0054	0.0242	2.0515
1.96	26.66	1.4993	0.2798	0.1021	0.0490	0.0274	0.0169	0.0112	0.0078	0.0056	0.0250	2.0241
2.56	33.43	1.3886	0.2600	0.0951	0.0457	0.0256	0.0158	0.0104	0.0073	0.0053	0.0234	1.8772
3.24	44.06	1.2630	0.2358	0.0862	0.0413	0.0232	0.0143	0.0096	0.0066	0.0048	0.0208	1.7056
4.00	54.40	1.1424	0.2123	0.0775	0.0372	0.0208	0.0128	0.0088	0.0059	0.0043	0.0189	1.5409
6.25	85.00	0.8919	0.1637	0.0595	0.0285	0.0160	0.0098	0.0064	0.0045	0.0033	0.0148	1.1984
9.00	122.40	0.7101	0.1290	0.0468	0.0224	0.0125	0.0077	0.0048	0.0035	0.0026	0.0117	0.9511
12.25	166.60	0.5780	0.1041	0.0377	0.0180	0.0100					0.0243	0.7721
16.00	217.60	0.4797	0.0858	0.0310	0.0148	0.0083					0.0201	0.6397
20.25	275.40	0.4050	0.0721	0.0260	0.0124	0.0069					0.0167	0.5391
25.00	340.00	0.3468	0.0614	0.0221	0.0105	0.0059					0.0142	0.4609
36.00	489.60	0.2634	0.0463	0.0166	0.0079	0.0044					0.0107	0.3493
49.00	666.40	0.2075	0.0363	0.0130	0.0062	0.0034					0.0084	0.2748
72.25	989.40	0.1526	0.0265	0.0095	0.0045	0.0025					0.0062	0.2018

TABLE II. Excitation cross sections of $n=2$ level to $n'=3$, 4, 5, 6, 7, 8 levels in units of πa_0^2.

Impact energy Ry	eV	$Q(2,3)$	$Q(2,4)$	$Q(2,5)$	$Q(2,6)$	$Q(2,7)$	$Q(2,8)$	$\sum_{m=9}^{\infty} Q(2,m)$	$Q(T)$
0.2025	2.75		7.385						
0.25	3.40		12.016	3.933	1.706	0.868	0.491	0.570	92.037
0.36	4.90	70.796	13.227	4.941	2.435	1.395	0.880	1.566	95.240
0.64	8.70	57.213	10.794	4.104	2.049	1.186	0.753	1.351	77.433
1.00	13.60	45.062	8.334	3.151	1.570	0.907	0.576	1.033	60.633
1.44	19.58	36.042	6.538	2.456	1.220	0.704	0.446	0.800	48.206
1.96	26.66	29.415	5.250	1.960	0.971	0.559	0.354		
2.56	33.43	24.462	4.309	1.601	0.791	0.455	0.288		
3.24	44.06	20.679	3.602	1.332	0.657	0.378	0.239	0.427	27.314
4.00	54.40	17.726	3.059	1.127	0.555	0.319	0.201		
4.84	65.82	15.386	2.632	0.968	0.475	0.272	0.173		
5.76	78.34	13.493	2.293	0.840	0.412	0.236	0.149		
6.76	91.94	11.927	2.016	0.737	0.361	0.207	0.131		
7.84	106.62	10.633	1.792	0.652	0.319	0.183	0.116		
9.00	122.40	9.547	1.596	0.582	0.284	0.163	0.103		

TABLE III. Excitation cross sections for the transition $n=3$ to $n'=4$, 5, 6, 7, 8, in units of πa_0^2.

Impact energy Ry	eV	$Q(3,4)$	$Q(3,5)$	$Q(3,6)$	$Q(3,7)$	$Q(3,8)$	$\sum_{m=9}^{\infty} Q(3,m)$	$Q(T)$
0.07	0.95	657.1						
0.08	1.1	709.2	83.37					
0.111	1.5	735.3	126.98	42.92	19.16	9.94	12.04	946.3
0.16	2.2	676.9	125.33	47.26	23.56	13.67	22.86	909.6
0.36	4.9	460.9	83.69	31.86	16.08	9.44	16.02	618.0
0.64	8.7	322.3	56.35	21.16	10.62	6.21	10.52	427.2
1.00	13.6	237.4	40.33	14.98	7.47	4.35	7.36	311.9
1.44	19.6	182.5	30.34	11.19	5.55	3.23		
1.96	26.7	145.1	23.69	8.69	4.29	2.49		
2.56	33.4	118.4	19.07	6.94	3.45	1.99		
3.24	44.1	98.5	15.71	5.70	2.81	1.62		
4.00	54.4	83.5	13.19	4.75	2.34	1.38	2.30	107.2
6.25	85.0	58.5	9.12	3.25	1.61	0.97		
9.00	122.4	43.6	6.71	2.38	1.19	0.66		

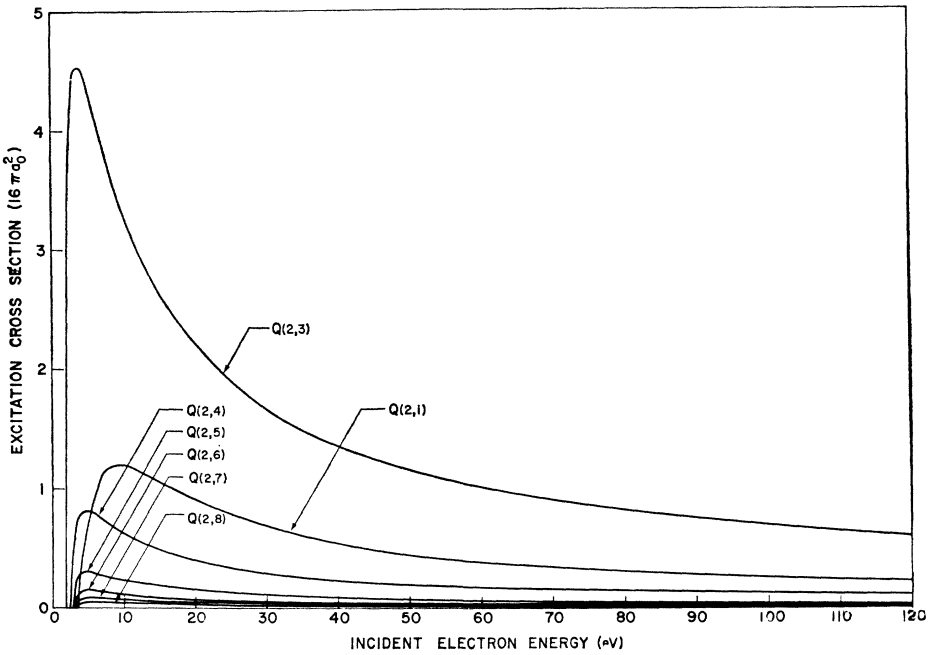

FIG. 3. Excitation of the $n=2$ states to the $n=3$, 4, 5, 6, 7, 8 states. $Q(2,i)$ is the averaged ionization cross section of the $n=2$ states.

the cross sections between sublevels in one system is equal to the same sum in the other system. This was verified. The excitation cross sections, averaged over the initial substates and summed over the final substates, for the initial states $n=1$ to 5 are listed in Tables I–V. For a given initial state n_i the cross section due to all higher states which are not listed explicitly is obtained by an interpolation method between excitation and ionization.[15] This is designated by

$$\sum_{m=n}^{\infty} Q(n_i,m),$$

where n is the upper state of the highest transition whose cross section is listed in the table. $Q(T)$ is the total excitation cross section for the transition between an initial state and all the higher states, excluding the continuum. The $Q(T)$ values are not given for some impact energies because of the unavailability of ionization values for these energies.

To test the accuracy of the Born approximation, it is necessary to compare the result of the Born calculation with experiment. This is done in Fig. 1; the more elaborate theoretical calculation of close coupling,[16] and the classical theory of excitation given by Gryzinski,[17] are also displayed.

When compared to experiment, the values given by the Born approximation are too high, those of the classical theory are too low, and those of the close-coupling approximation are in the best agreement. It

TABLE IV. Excitation cross sections for the transition $n=4$ to $n'=5$, 6.

Impact energy		$Q(4,5)$	$Q(4,6)$	$\sum_{m=7}^{\infty} Q(4,m)$	$Q(T)$
Ry	eV	πa_0^2	πa_0^2	πa_0^2	πa_0^2
0.03	0.41	3081			
0.04	0.54	3778	432.4		
0.0625	0.85	3795	660.1	549	5004
0.111	1.51	3137	570.5		
0.16	2.18	2584	462.1	475	3521
0.36	4.90	1567	264.3	269	2100
0.64	8.70	1050	169.7	171	1391
1.00	13.6	759	118.6	119	997
1.44	19.6	581	88.1		
1.96	26.7	450	68.5		
2.56	33.4	367	54.3		
3.24	44.1	306	44.6		
4.00	54.4	262	37.4		
6.25	85.0	190	25.9		
9.00	122.4	151	19.4		

[15] For a description of this method see Ref. 4.

TABLE V. Excitation cross sections for the transition $n=5$ to $n'=6$ in units of πa_0^2.

Impact	Ry	0.0169	0.0225	0.04	0.111	0.16
energy	eV	0.23	0.31	0.54	1.51	2.18
$Q(5,6)$	πa_0^2	11308	13792	13588	8698	6889
Impact	Ry	0.36	0.64	1.00	1.44	1.96
energy	eV	4.90	8.70	13.6	19.6	26.7
$Q(5,6)$	πa_0^2	3980	2628	1907	1485	1221
Impact	Ry	2.56	3.24	4.00	6.25	9.00
energy	eV	33.4	44.1	54.4	85.0	122.4
$Q(5,6)$	πa_0^2	1048	929	845	719	654

[16] K. Omidvar, Phys. Rev. **133**, A970 (1964). For numerical results of the Born approximation see K. Omidvar, NASA TN D-2145, Goddard Space Flight Center, Greenbelt, Maryland (unpublished). Also see P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962).

[17] M. Gryzinski, Phys. Rev. **115**, 374 (1958). An improved calculation of Gryzinski has been performed by R. Stabler, Phys. Rev. **133**, A1264 (1964); see also V. I. Ochkur and A. M. Petrunkin, Opt. Spectry. **14**, 245 (1963).

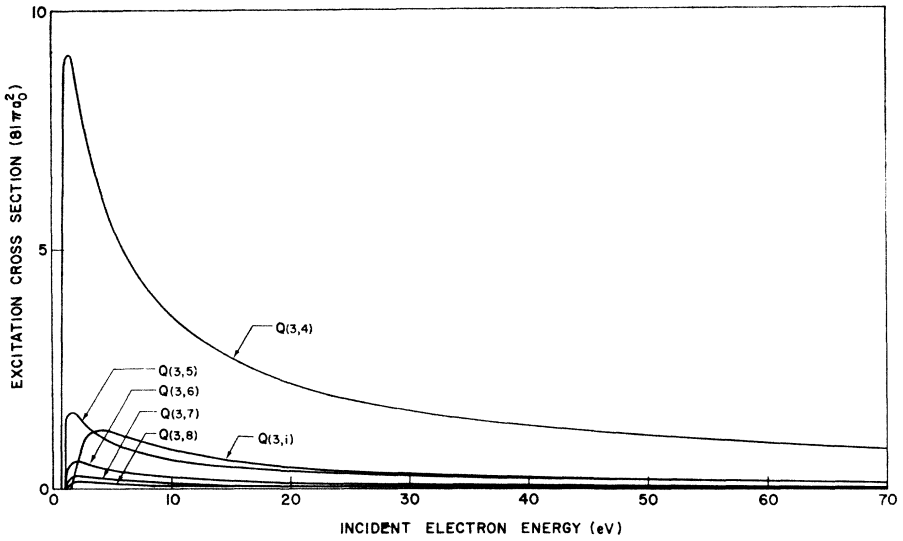

FIG. 4. Excitation of the $n=3$ states to the $n=4$, 5, 6, 7, 8 states. $Q(3,i)$ is the averaged ionization cross section of the $n=3$ states.

should be emphasized that the classical description of the excitation is open to question, as transitions to discrete levels cannot be described classically. Furthermore, according to this theory all the degenerate levels have the same cross sections.

The disagreement between Born calculations and experiment may get worse for excitation of the higher states. This is due to the form of the wave function of the bound electron. Since a hydrogenic wave function is used to evaluate the matrix elements of the Born approximation, it is implicitly assumed that the interaction potential between the two electrons is small compared with the interaction of the nucleus and the atomic electron. This, however, may not be the case for the excited states where the average distance of the electron from the nucleus is large.

Figure 2 compares different excitation and ionization cross sections for the $n=1$ level. Figures 3 and 4 make the same comparison for the $n=2$ and the $n=3$ levels. Figures 5 and 6 correspond to excitation of $n=4$ and 5. It is interesting to note that the ionization cross section of the level n, compared to its excitation cross section, becomes progressively smaller as n increases.

A remark should be made about the relative magnitudes of cross sections for optically allowed and non-optically-allowed transitions. For low-lying levels, the

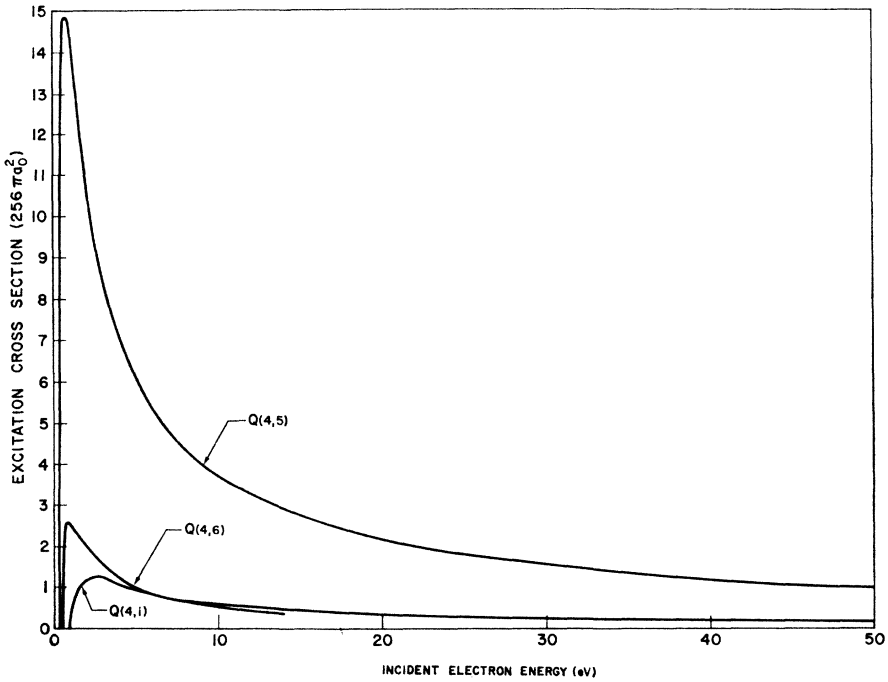

FIG. 5. Excitation of the $n=4$ states to the $n=5$, 6 states. $Q(4,i)$ is the averaged ionization cross section of the $n=4$ states.

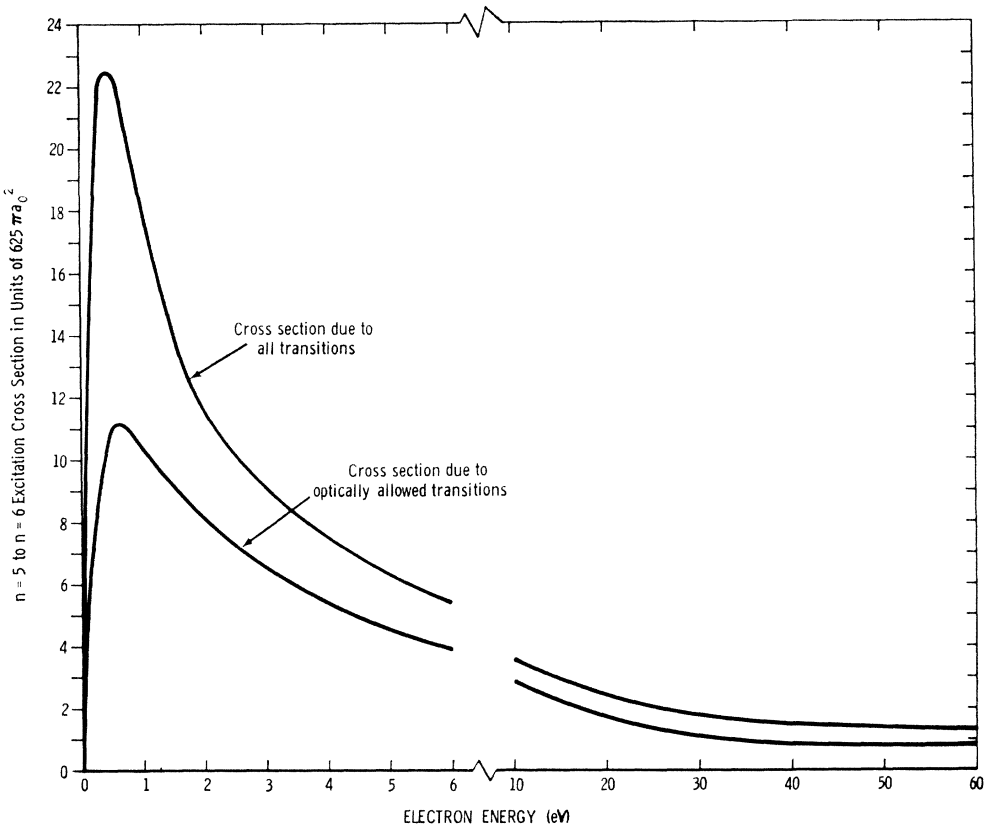

FIG. 6. Excitation of the $n=5$ states to the $n=6$ states. The cross section due to optically allowed transitions is given for comparison.

optically allowed transitions have cross sections larger by an order of magnitude than the non-optically-allowed, as is evidenced by comparison of the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ cross sections.[16] For highly excited states the cross sections due to non-optically-allowed transitions become appreciable for two reasons: (I) the contribution of higher terms of expansion of $\exp[iKz]$ compared to Kz in the integrand of the excitation amplitude becomes larger as the radius of the atom increases in excited states, and (II) the statistical weight of non-optically-allowed transitions compared with optically allowed ones becomes larger for excited states. The total number of transitions between n and n' is given by (27), compared with n^2 for the number of optically allowed transitions. For high n the optically allowed transitions contribute a fraction of $[n'-(n/3)]^{-1}$ to the total number of transitions. In Fig. 6 comparison is made of the two types of transitions. The sharp peak of the total-transitions curve is the result of the inclusion of the optically forbidden transitions.

Knowing the cross sections for excitation to all levels and for ionization, curves can be constructed which show total inelastic cross sections (excluding de-excitations) for different levels. This is shown in Fig. 7 for $n=1$, 2, 3, 4, and 5.

The de-excitation process $Q(f,i)$ is related to the excitation process $Q(i,f)$ by

$$Q(f,i)=(k_i/k_f)^2 Q(i,f), \tag{28}$$

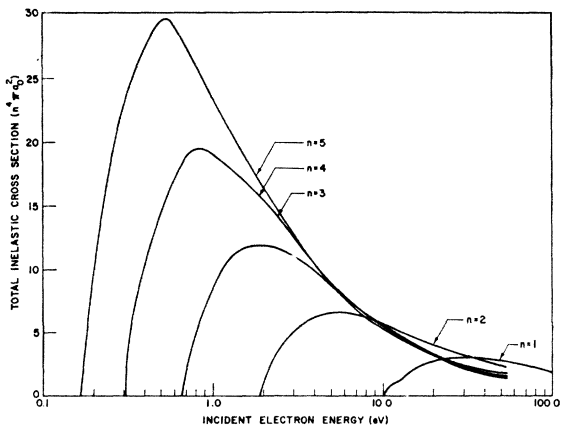

FIG. 7. Total inelastic cross section, including excitation to all states and ionization, of the hydrogen atom for electron collision. Different curves correspond to the atom initially in the states $n=1$, 2, 3, 4, and 5.

with k_i and k_f the initial and final wave numbers in the excitation process.

In a calculation which will be reported later the present calculation will be extended to higher excited states and to higher energy ranges, and exchange of the electrons will be included.

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Radiative Cascade Theory

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A steady-state cascade theory has been set up for radiative electron transitions. These are assumed to occur between a continuum and various excited states, as well as between any two excited states, of hydrogen-like atoms. The work contains two features which have not previously been fully taken into account: (1) Both spontaneous and induced transition probabilities have been included exactly. (2) In addition to the radiative transitions, the reverse transitions due to absorption of background radiation have also been included. The following graphical results are given: (a) The steady-state occupation probabilities of the excited states as a function of excess electron density. (b) A "sticking probability" P_n (for an electron from a level n to reach the ground state without leaving the atom) as a function of the principal quantum number n. (c) The effect of the cascade on the transition rate into the ground state. The calculation is valid for semiconductors and for the analogous astrophysical problem. Temperature dependences have also been studied. The graphs shown bear out quantitatively the expectation that P_n decreases as either the temperature or the principal quantum number increases.

1. INTRODUCTION

RECOMBINATION-generation processes involving a series of levels (e.g., excited atomic states) lead automatically to cascade problems. In these, electrons can move up and down the energy scale and the transition probabilities between any two levels, together with the assumption of a steady state, leads to a steady non-equilibrium probability distribution for the occupation of the quantum states involved. This will in general differ from the cruder "quasi-Fermi" distribution often hypothesized in solid-state work.

The simplest cascades are those involving a conduction band (a continuum in astrophysics) and the states, labeled by the principal quantum number n, of hydrogen-like ions. In such cases the results of the calculation may be given in terms of the probabilities Π_n that an electron will reach the ground state from level n without leaving the atom. This has been called the "sticking probability" in solid-state work, and has proved difficult to calculate. If states lying above $n=N$ are neglected an approximate probability $\Pi_{n,N}$ is obtained. Many results of this paper are presented in terms of "reduced" sticking probabilities $P_{n,N}$. As far as we are aware, this is the first time this probability has been investigated systematically for a solid-state problem by a quantum-mechanical method.

The assumptions made in this paper are: the electrons in the band having a Maxwell distribution in the steady state; hydrogen-like wave functions for the discrete and continuum states, modified by an effective mass and a dielectric constant; black-body radiation in the solid; Saha dissociation formula for equilibrium even for the large principal quantum numbers n; neglect of term structure for given n. If the steady state is maintained by pumping electrons back into the continuum a general theory is readily set up [Eq. 4.2(a)]. If it is also assumed that all transitions are radiative, the matrix elements which occur are standard. For the purposes of numerical calculations the problem can be further simplified by supposing that because the lowest level $n=1$ is the most highly populated of the discrete levels, the pumping action may be neglected for the levels $n \geqslant 2$. This leads to the final set of Eqs. (5.17) whose solutions are readily computed.

The cascade model set up in this way is informative in spite of the limitations implied by the above assumptions. It provides guiding lines for a more complete cascade theory which incorporates also the effect of phonons and of electron collisions, but such a theory is not attempted here.

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