BORN CROSS-SECTIONS FOR SELECTED INELASTIC COLLISIONS OF PROTONS WITH HYDROGEN ATOMS IN STATES UP TO $n = 10$*

JOHN CAREW
St. John's University, Jamaica, New York

AND

S. N. MILFORD
Research Department, Grumman Aircraft Engineering Corporation, Bethpage, New York

Received April 25, 1963

ABSTRACT

Born total cross-sections for inelastic collisions of protons with excited hydrogen atoms may be derived approximately from the Born cross-sections for inelastic collisions of electrons with excited hydrogen atoms. A comparison of the exact and approximate Born cross-sections for the collisions $p + H(nl) \rightarrow p + H(n'l')$: 1s–2s, 1s–2p, 3s–4p, 3d–4f, shows that they agree down to energies near the Born maximum. By using the known electron cross-sections, approximate Born total cross-sections are calculated for proton collisions for some of the transitions 1–n'; 2–n'; 3–4, 5; 4–5, 6; 5–6; 10–11. In addition, a simple formula is given for finding other approximate proton cross-sections in terms of the approximate electron cross-sections calculated recently.

I. INTRODUCTION

In order to consider in detail the state of excitation and ionization of high-temperature gases and plasmas which occur in laboratory or astrophysical situations where thermal equilibrium does not prevail, it is necessary to know all the relevant cross-sections and transition probabilities. While Born cross-sections for the ground state of hydrogen have been known for many years and extensive calculations of more accurate cross-sections for the ground state have now been carried out, it is only recently that cross-sections for (electron) collisions with excited atoms have been calculated.

The present paper extends these cross-section calculations to inelastic *proton* collisions with excited hydrogen atoms. Because the Born proton cross-sections can be determined rather easily from the Born electron cross-sections, it was decided to limit these calculations to the various 1–n'; 2–n'; 3–4, 5; 4–5, 6; 5–6; 10–11 transitions for which electron cross-sections are available. In previous investigations by Bates and Griffing (1953), the Born approximation for inelastic proton collisions with ground-state hydrogen atoms has been discussed for the transitions 1s–2s, p; 3s, p, d; continuum (for other approximations see Bates 1962).

II. CROSS-SECTION FORMULAE

The differential cross-section for the excitation of hydrogen by impact of a bare nucleus of charge Ze is given in the first Born approximation by

$$\sigma_{nn'}{}^{+}(K^{+})\, dK^{+} = \frac{8\pi M^2 Z^2 e^4}{(k_n{}^{+})^2 \hbar^4} \left| J_{nn'}(K^{+}) \right|^2 \frac{dK^{+}}{(K^{+})^3}, \tag{1}$$

where

$$J_{nn'}(K) = \int e^{iKZ} \psi_n(\mathbf{r}) \psi_{n'}{}^{*}(\mathbf{r})\, d\mathbf{r} \tag{2}$$

* Supported in part by the Air Force Office of Scientific Research under grants AF 61-10 and 61-20, and by the Office of Naval Research under contract NR012-106, to St. John's University.

Based in part on a thesis submitted by John Carew to the graduate school of St. John's University in partial fulfilment of the requirements for the degree of Master of Science.

and M is the reduced mass of the hydrogen atom and the incident bare nucleus, $\hbar \mathbf{k}_n^+$ is the initial relative momentum vector, and $\hbar \mathbf{K}^+$ is the change in relative momentum of the hydrogen atom and the incident nucleus.

The differential cross-section for the corresponding electron hydrogen atom collision is given by

$$\sigma_{nn'}^-(K^-)\,dK^- = \frac{8\pi m^2 e^4}{(k_n^-)^2\hbar^4}\,|J_{nn'}(K^-)|^2 \frac{dK^-}{(K^-)^3}, \tag{3}$$

where m is the (reduced) electron mass, $\hbar \mathbf{k}_n^-$ is the initial momentum vector, and $\hbar \mathbf{K}^-$ is the change in (relative) momentum of the incident electron.

Following Bates and Griffing (1953), setting $K^+ = K^- = K$ and comparing equations (1) and (3), a relation between the electron and proton differential cross-sections follows:

$$\sigma_{nn'}^+(K) = \left(\frac{M k_n^-}{m k_n^+}\right)^2 \sigma_{nn'}^-(K)\,. \tag{4}$$

Thus the total proton cross-section can be expressed in terms of the differential electron cross-section

$$\sigma_{nn'}^+(k_n^+) = \left(\frac{M k_n^-}{m k_n^+}\right)^2 \int_{K_{\min}^+}^{K_{\max}^+} \sigma_{nn'}^-(K)\,dK\,, \tag{5}$$

while the total electron cross-section is

$$\sigma_{nn'}^-(k_n^-) = \int_{K_{\min}^-}^{K_{\max}^-} \sigma_{nn'}^-(K)\,dK\,. \tag{6}$$

By setting $K_{\min}^+ = K_{\min}^-$ (which imposes condition [9] below on the electron and proton energies), an exact equality is

$$\sigma_{nn'}^+(k_n^+) = \left(\frac{M k_n^-}{m k_n^+}\right)^2 \left[\sigma_{nn'}^-(k_n^-) + \int_{K_{\max}^-}^{K_{\max}^+} \sigma_{nn'}^-(K)\,dK\right]. \tag{7}$$

While, in general, $K_{\max}^+ \gg K_{\max}^-$, for moderate energies both quantities are large enough that the integral in equation (7) is very small, leading to the approximate result:

$$\sigma_{nn'}^+(k_n^+) \approx \left(\frac{M k_n^-}{m k_n^+}\right)^2 \sigma_{nn'}^-(k_n^-)\,. \tag{8}$$

In setting the lower limits equal, Bates and Griffing pointed out that it is usually sufficient to take $K_{\min}^+$ as $M\Delta E/\hbar^2(k_n^+)^2$, where ΔE is the threshold energy for $n \rightarrow n'$, while the exact expression is necessary for $K_{\min}^-$. It follows that the electron and proton energies will be related as follows:

$$M^2(k_n^-)^2 = \gamma m^2 (k_n^+)^2\,, \qquad \gamma = \left\{1 + \frac{M^2 \Delta E}{2 m \hbar^2 (k_n^+)^2}\right\}^2, \tag{9}$$

and the approximate proton cross-section (8) becomes

$$\sigma_{nn'}^+(k_n^+) \approx \gamma\,\sigma_{nn'}^-(k_n^-)\,. \tag{10}$$

In the present paper, it will be shown that the approximate cross-section (10) reproduces the Born cross-sections quite well in the energy regions where the latter are accurate, and then formula (10) will be used to compute a number of approximate proton cross-sections.

III. RESULTS

In order to determine the accuracy of the approximate cross-section formula (10), a comparison was made of the values calculated by formula (10) and the actual Born cross-sections. Throughout the present paper, all cross-sections have been averaged over the initial magnetic quantum number m and summed over the final m'. The Born 1–2 transition values are given by Bates and Griffing (1953); the Born cross-sections for the 3s–4p and 3d-4f transitions were calculated from equation (5) and the available electron differential cross-sections (McCoyd, Milford, and Wahl 1960) and are listed in Table 1. The total electron cross-sections that were used in the approximate Born

TABLE 1

COMPARISON OF EXACT AND APPROXIMATE BORN CROSS-SECTIONS FOR 3s–4p AND 3d–4f TRANSITIONS (IN UNITS OF πa_0^2)

C.M energy (kev) . .	0 54	2 63	53 41	1257
Exact Born: 3s–4p	66	133	31 51	2 583
C.M. energy (kev) .	0 542	2 68	54 21	1252
Approximate Born: 3s–4p	65 1	133	31 19	2 599
C.M. energy (kev)	0 299	2 17	2 68	54 21
Exact Born: 3d–4f .	615	658	603	85 25
Approximate Born: 3d–4f	570	658	603	85 25

TABLE 2

APPROXIMATE TOTAL BORN CROSS-SECTIONS FOR 2–3 TRANSITIONS (IN UNITS OF πa_0^2)

C M Energy (kev)	2s–3s	2s–3p	2s–3d	2p–3s	2p–3p	2p–3d
0 542	10 9	0 27	46	2 0	13 7	31
0 964	22	6 2	86	3 3	26	71
1 190	. .	9 6	. .	3 0	.	78
1 388	21 4	12 18	80 6	2 70	25 7	80 7
1 640	20 5	. . .	75 2	. . .	24 3	. . .
2 17	18 3	18 5	64 8	1 87	21 3	82 1
8 67	6 72	20 5	21 9	0 771	7 49	52 2
34 7	1 85	10 70	5 89	0 348	2 04	22 5
138 8	0 475	4 19	1 50	0 1333	0 520	8 08
867	0 0765	1 000	0 242	0 0315	0 0837	1 82

formula are given in several sources (Massey 1956; McCarroll 1957; McCoyd *et al.* 1960; Scanlon and Milford 1961). The comparisons between the Born and the approximate Born cross-sections for the proton collisions are presented in Figure 1. The agreement is excellent right down to the Born maximum for the 3–4 transitions and is believed to be equally good for the 1–2 transitions—for the latter, approximate values for the Born cross-sections were read from the Bates and Griffing graphs. It appears, then, that Born cross-sections for proton collisions can be calculated with sufficient accuracy from the simple approximate Born formula (10).

Using the approximate formula and all available electron hydrogen atom Born total cross-sections (Massey 1956; McCarroll 1957; Boyd 1958; McCoyd *et al.* 1960; Fisher, Milford, and Pomilla 1960; Milford, Morrissey, and Scanlon 1960; Scanlon and Milford 1961; McCoyd and Milford 1963), the corresponding proton hydrogen atom approximate Born total cross-sections were calculated. The results are given in Tables 2 and 3.

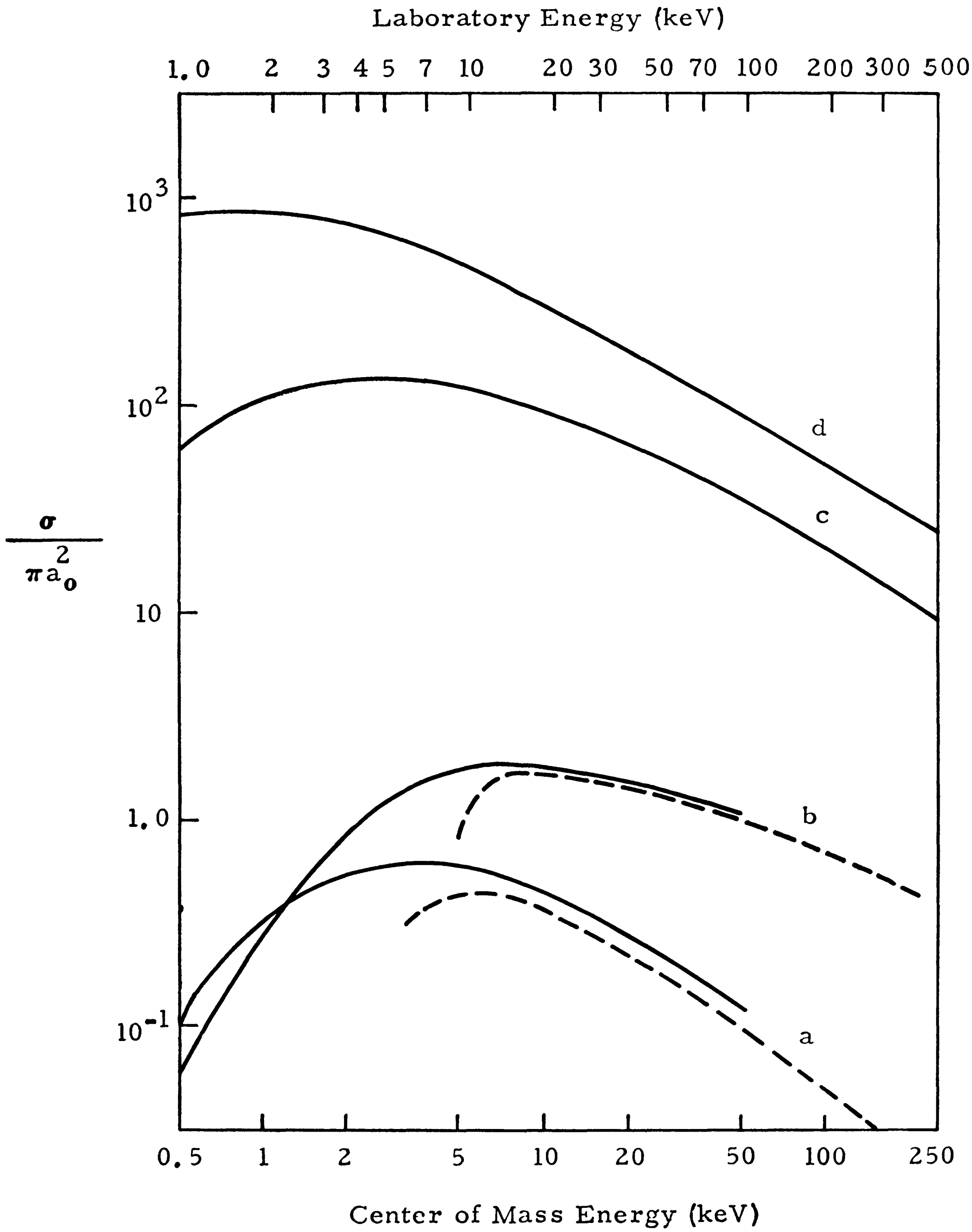

FIG. 1 —Comparison of exact Born (*solid curves*) and approximate Born (*broken curves*) total cross-sections for the 1s–2s, 1s–2p, 3s–4p, and 3d–4f hydrogen atom transitions produced by proton impact: (*a*) 1s–2s; (*b*) 1s–2p; (*c*) 3s–4p; (*d*) 3d–4f. Note that the exact and approximate Born curves for the 3s–4p and 3d–4f transitions merge together on this scale.

IV. DISCUSSION

At high energies $\gamma \sim 1$, and the well-known result follows: the proton and electron cross-sections are equal at high energies for equal incident velocities of the proton and the electron.

Also, within the present approximation, the proton and electron cross-sections have the same behavior with respect to the optical strength of transitions: the largest cross-sections are for optically allowed transitions in which n and l change in the same sense.

TABLE 3

APPROXIMATE TOTAL BORN CROSS-SECTIONS FOR VARIOUS 3–4, 5; 4–5, 6; 5–6; AND 10–11 TRANSITIONS (IN UNITS OF πa_0^2)*

Transition	C.M. Energy (kev)				
	0 297	0 542	2.17	12.45	110 6
3s–4s	15 (1)	190	103	22 0	2 57
3s–4p	7 (1)	65	133	79 4	18 5
3s–4d	27 (1)	385	210	44 9	5 25
3s–4f	62 (1)	475	135	23 9	2 69
3p–4s	56	36	12 5	5 44	1 233
3p–4p	19 (1)	238	122	26 0	3 04
3p–4d	11 (1)	193	259	121 9	26 0
3p–4f	66 (1)	646	259	51 4	5 93
3d–4s	7 5	6 9	2 53	0 524	0 0612
3d–4p	57	42	12 2	3 17	0 566
3d–4d	23 (1)	239	104	21 1	2 44
3d–4f	57 (1)	785	658	250	48 5
	0 617	2 47	3 86	18 02	8882
3s–5p	10	21 9	21 5	11 16	0 0816
3p–5d	31	43 0	37 6	16 1	0 1007
3d–5f	11 (1)	85 5	67 9	24 1	0 1259
	0 347	1 388	3 12	15 81	1249
4s–5p	3 (2)	522	460	203	6 76
4p–5d	6 (2)	797	630	253	7 90
4d–5f	133 (1)	150 (1)	1101	409	12 06
4f–5g	42 (2)	325 (1)	215 (1)	721	19 5
	0 542	1 388	2 17	8 67	3470
4s–6p	6 (1)	8 (1)	8 (1)	48	0 46
4f–6g	52 (1)	393	309	120 9	0 757
	0 326	0 656	1 041	12 14	48 6
5s–6p	. .	16 (2)	16 (2)	56 (1)	21 (1)
5p–6d	1 (3)	21 (2)	20 (2)	63 (1)	23 (1)
5d–6f	2 (3)	35 (2)	33 (2)	92 (1)	33 (1)
5f–6g	66 (2)	66 (2)	582 (1)	141 (1)	490
5g–6h	16 (3)	134 (2)	1103 (1)	227 (1)	762
	1032 3	16516			.
10s–11p	223	18 5			.
10, 9–11, 10	924	73 9	.		. .

* The numbers in parentheses represent powers of 10

Approximate Bethe cross-sections (McCoyd and Milford 1963) are now available for electron collisions with hydrogen atoms for the transitions $\Delta n = +1, +2$ and $\Delta l = +1$, for $n = 1$–10. In order to use these results for proton collisions with hydrogen atoms, it is noted that the Bethe (dipole) electron cross-section is

$$\begin{aligned}\sigma^{-D} &= \frac{18.14}{E^-}\left(\frac{l+1}{2l+1}\right)\left|\frac{I(n, l \rightarrow n', l+1)}{a_0}\right|^2 ln\left[\frac{54.42(K_c a_0)^2 E^-}{(\Delta E)^2}\right]\pi a_0^2 \\ &= \frac{C}{E^-} ln(DE^-)\pi a_0^2 ,\end{aligned} \tag{11}$$

where E^- is the relative electron energy in electron volts, a_0 is the radius of the first Bohr orbit, $|I/a_0|^2$ is the square of the radial integral in the dipole moment matrix element and is tabulated by Green, Rush, and Chandler (1957), and $\hbar K_c$ is the cutoff momentum in the center-of-mass system. With the same procedure as that used in deriving equation (10), the relation between the dipole cross-sections is

$$\sigma^{+D}(E^+) = \gamma \sigma^{-D}(E^-) \tag{12}$$

$$= C\frac{\gamma}{E^-} ln(DE^-)\pi a_0^2 . \tag{13}$$

The quantities C and D are given by McCoyd and Milford (1963, Tables IV and V) and enable the proton dipole cross-sections to be calculated very quickly; E^+ is the relative proton energy in electron volts.

For those hydrogen transitions for which no electron cross-sections have been calculated, it is possible to use the simple approximate formulae recently developed for both allowed (Milford 1960) and forbidden (Scanlon and Milford 1961) transitions induced by electron impact, provided that the corresponding multipole moments are known. The approximate proton cross-sections then follow from the approximate electron cross-sections via equation (10).

It is interesting to note the relative magnitudes of the proton and electron cross-sections at various energies. In typical laboratory or astrophysical plasmas the temperatures are in the range 1–1000 ev, so that, for the lower states of hydrogen, the proton cross-sections are small compared with the electron cross-sections in the range where the Maxwell-Boltzmann velocity distribution peaks. However, for the higher states of hydrogen (say $n = 10$–30) the electron cross-sections peak at energies of about 0.001–0.1 ev, compared with proton cross-sections with maxima in the range 1–100 ev, so that, for some higher states, the proton collisions dominate the electron collisions.

We would like to thank Dave Bouthilette for checking the calculations and Joe Scanlon and Gerard McCoyd for discussions.

REFERENCES

Bates, D. R. 1962, *Atomic and Molecular Processes*, ed. D. R. Bates (New York: Academic Press), chap. 14.
Bates, D. R., and Griffing, G. W. 1953, *Proc. Phys. Soc. London*, A, **66**, 961.
Boyd, T. J. M. 1958, *Proc. Phys. Soc. London, A*, **72**, 523.
Fisher, L., Milford, S. N., and Pomilla, F. R. 1960, *Phys. Rev.*, **119**, 153.
Green, L. C., Rush, P. P., and Chandler, C. D. 1957, *Ap. J. Suppl.*, **3**, 37.
McCarroll, R. 1957, *Proc. Phys. Soc. London, A*, **70**, 460
McCoyd, G. C., and Milford, S. N. 1963, *Phys. Rev.*, **130**, 206.
McCoyd, G. C., Milford, S. N., and Wahl, J. J. 1960, *Phys. Rev.*, **119**, 149.
Massey, H. S. W. 1956, *Hdb. d. Phys.*, ed. S. Flügge (Berlin: Springer-Verlag), **36**, 354
Milford, S. N 1960, *Ap. J.*, **131**, 407.
Milford, S N., Morrissey, J. J., and Scanlon, J. H. 1960. *Phys. Rev.*, **120**, 1715.
Scanlon, J H., and Milford, S. N. 1961, *Ap. J*, **134**, 724.