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CROSS SECTIONS FOR COLLISIONS OF ELECTRONS WITH HYDROGEN ATOMS AND HYDROGEN-LIKE IONS

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A B S T R A C T

On the basis of a limited critical review of present theory and experiment, cross sections are recommended for the ionization of any level of hydrogen or any hydrogenic ion by electrons, for the excitation of any level from the ground level, and $n \rightarrow n + 1$ excitation from higher levels. Individual angular momentum and Stark states of the levels are not considered.

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INTRODUCTION

For high energies of the incoming electron the Born approximation is valid. As the energy decreases, and particularly in the neighbourhood of the peak cross section for a given process, the Born approximation to the cross section is usually too big, and we rely on very few experimental results for ionization and excitation, together with theoretical estimates of relative cross sections for different processes and approximations, to obtain recommended cross sections for a wide variety of processes, most of which are inaccessible to direct experiment. If any of these experimental results should prove to be seriously in error, then all our estimates based on them would be similarly in error in the region where the Born approximation is invalid.

The relative cross sections are obtained by estimating factors of three types:

(1) Correction factors. These are the factors by which we must multiply the Born or Bethe cross sections to obtain the correct cross section. They are usually less than unity, but tend to unity for high energy.

(2) Scaling factors for n. These are the factors by which we obtain an approximate cross section for arbitrary principal quantum number n from the cross section for $n = 1$ or $n = 2$. Both the cross section and the energy scale must be altered.

(3) Coulomb factors. These are the factors by which we obtain an approximate cross section for arbitrary nuclear charge Z from that for $Z = 1$ or $Z = 2$. Again both cross section and energy are changed.

The form of these factors is chosen empirically, using various theories as a guide. We are prepared to tolerate additional errors of a few per cent in the cross sections in order to simplify the factors.

NORMALIZED CROSS SECTIONS

Cross sections σ are given in units of $\pi a_0^2 = 0.88 \times 10^{-16}$ cm^2. The suffix B represents a Born cross section, suffix X an experimental cross section and suffix R a recommended cross section. The energy E is the energy of the incoming electron, given in eV, and U is the ionization energy of the initial state of a collision. The ratio

$$\frac{E}{U} = \tilde{E} \qquad \dots (1)$$

defines the normalized energy $\tilde{E}$. In the case of collision of an electron with the ground state of neutral hydrogen $\tilde{E}$ is the energy in Rydbergs. For a collision with an arbitrary level n of a hydrogenic ion of nuclear charge Z, the unit of energy for $\tilde{E}$ is $(Z/n)^2$ Ry.

The (harmonic) mean radius of all the n^2 states of a hydrogen atom ($Z = 1$) of level n is

$$a_n = n^2 a_o \qquad \ldots (2)$$

and we may therefore define a mean effective surface area as

$$S_n = \pi a_n^2 = n^4 \pi a_o^2 \,. \qquad \ldots (3)$$

For a hydrogen atom the ratio

$$\tilde{\sigma} = \pi a_o^2 \, \sigma / S_a = n^{-4} \sigma \qquad \ldots (4)$$

defines $\tilde{\sigma}$. This is called a normalized cross section when expressed as a function of the normalized energy $\tilde{E}$. Normalized cross sections are much easier to compare than the original cross sections.

The choice of a normalization factor to relate cross sections for different Z is not so simple. The harmonic mean radius is

$$a_{nz} = n^2 Z^{-1} a_o$$

but the effective cross sections measured in units of πa_{nz}^2 are not comparable. The reason is that in order for a transition to take place the electron-electron interaction has to compete with the electron-nucleus interaction, which tends to keep the bound electron in its initial state. On a crude classical picture we should expect the electron-electron interaction to dominate over a fraction Z^{-2} of the total effective area. This suggests that the normalized cross section should be

$$\begin{aligned} \tilde{\sigma} &= \pi a_o^2 \, \sigma Z^2 / (\pi a_{nz}^2) \\ &= (Z/n)^4 \, \sigma \end{aligned} \qquad \ldots (5)$$

This is a good basis for the initial comparison of cross sections with different Z.

If the initial state is a ground state of the hydrogen atom

$$\tilde{\sigma}(\tilde{E}) = \sigma(E/1\text{Ry}) \qquad \ldots (6)$$

The cross section from a given level n is the average cross section from all states of that level.

$$\sigma_n = \sum \sigma_{i_n} \qquad (\text{all } n^2 \text{ states } i_n) \qquad \ldots (7)$$

It is the effective cross section when all n^2 states are initially equally populated. The cross section to a given level is the sum over cross sections to all states of that level. The spins of the electron and the nucleus are neglected.

IONIZATION CROSS SECTIONS FOR NEUTRAL HYDROGEN

The experimental results of Fite and Brackmann (1958) for ionization from the ground level have been largely confirmed by Boyd and Boksenberg (1959) and by Rothe et al. (1962). We use the results of Boyd and Boksenberg as a standard of comparison for the recommended ionization cross sections. The data is taken from the report of Kieffer (1965)*. According to the other experiments these results could be too small by as much as 10% at peak cross section. The ionization cross section at peak is not known any better than this, as below 120 eV incident energy the theories are probably less reliable than the experiments.

For higher energies we may use the Born cross sections of Massey and Mohr, discussed by Massey (1956), but at still higher energies even this approximation requires a considerable amount of numerical work, and it is better to use Bethe's (1930) approximation, as described by Mott and Massey (1949) p.247, and Seaton (1962a). This gives the two leading terms in the asymptotic expansion of the cross section.

$$\sigma \sim \frac{1}{\tilde{E}} (A \ln \tilde{E} + B) \qquad \ldots (8)$$

The coefficient A depends only on the optical properties of the atom, which are well tabulated. The coefficient B is more difficult to obtain in general, but is given by Bethe for neutral hydrogen. Although the first term dominates for sufficiently high energies, these energies may be very high indeed. In the present case:

$$A = 1.14 \qquad B = 5.05 \qquad \ldots (9)$$

and the terms are equal when $E \approx 2$ keV.

To obtain an analytic formula for all energies we use the Bethe approximation as a basis for the following empirical recommended cross section, which does not differ from experimental or Bethe cross sections by more than 5% in their respective regions of validity:

$$\sigma_R(\tilde{E}) = \frac{(1.19 \ln \tilde{E} + 5.26)\,(\tilde{E} - 1)}{\tilde{E}^2 + 1.67\,\tilde{E} + 3.57} \qquad \ldots (10)$$

Ionization, $Z = 1$, $n = 1$. $\tilde{E} = E/1\mathrm{Ry}$

The recommended and experimental cross sections are compared in Fig.1.

Omidvar (1964) has obtained the Born ionization cross sections for the levels n = 1-5 and for the Stark states of these levels†. He also summarizes earlier work on Born cross

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* We multiply by a factor of 10 to compensate for an error in that report.

† There appears to be an error in the tabulated values for n = 5.

sections for ionization of hydrogen atoms. For sufficiently high n the normalized cross section $\tilde{\sigma}_n$ tends to the classical value for a fixed value of the normalized energy $\tilde{E} = \tilde{E}_n = n^2E/1Ry$. The normalized Born cross-sections for n = 1-4 do not differ substantially as a function of E up to $\tilde{E} \approx 6$, where the logarithmic term in the Bethe cross section becomes significant for n = 1. We shall suppose that the actual normalized cross sections do not differ substantially in the low energy region either, and that the major differences appear for large E where the Bethe approximation can be applied. We use the tables of Bethe and Salpeter (1957) to obtain the coefficients A, which are given by $1.28\ n^{-1}$ to a very good approximation for n = 2,3,4 and which we suppose to be valid for all n > 1. The coefficients B give more trouble. Here we can use the correspondence principle, that for fixed $\tilde{E}$, the cross section becomes classical in the limit as $n \to \infty$. We can the use the original classical asymptotic form of Gryzinski (1959)

$$\tilde{\sigma} \sim 6.67/\tilde{E} \qquad \ldots (11)$$

Therefore, the asymptotic form of the normalized cross section is given by

$$\tilde{\sigma}\ \tilde{E} \sim 1.28n^{-1}\ \ln \tilde{E} + 6.67 - q_n \qquad \ldots (12)$$

where $q_n \to 0$ as $n \to \infty$. By fitting to Omidvar's Born calculations we obtain for n > 1

$$\tilde{\sigma}\,\tilde{E} \sim 1.28n^{-1}\ \ln(\tilde{E}n^{-2}) + 6.67 \qquad \ldots (13)$$

and the following empirical form is recommended for the cross section:

$$\tilde{\sigma}_R(\tilde{E}) = \frac{[1.28n^{-1}\ \ln(\tilde{E}n^{-2}) + 6.67]\ [\tilde{E} - 1]}{\tilde{E}^2 + 1.67\ \tilde{E} + 3.57} \qquad \ldots (14)$$

Ionization, Z = 1, $n \geqslant 2$. $\tilde{E} = n^2\ E/1Ry$. $\sigma = n^4\ \tilde{\sigma}$

As n increases the logarithmic term tends to zero as n^{-1}, whilst the peak in the cross section tends to lower energies.

According to the Born calculations the ionization cross section does not depend critically on the ℓ state of the initial level when the cross section is near maximum. The Bethe approximation gives comparatively big differences between those states for the very high energies, where the logarithmic term dominates.

As shown by Rudge and Seaton (1965), at the threshold the ionization cross section is linear in E, unlike the Born approximation, which follows an $E^{3/2}$ law very close to threshold. Our recommended cross section has the correct behaviour, but it is doubtful if we can rely on the accuracy of the numerical values in the immediate neighbourhood of threshold.

Rudge and Seaton give references to the general theory of hydrogen atom ionization including the extensive work of Peterkop.

IONIZATION CROSS SECTIONS FOR HYDROGENIC IONS

The experimental results for ionization from the ground level of He^+ given by Dolder, Harrison and Thonemann (1961) are approached as the theories are improved, as we see for example in the work of Taylor and Burke (1964) and of Burgess (1964).

The simplest assumption we can make is that the normalized cross section for ionization of the ground state is independent of Z, for $Z \geqslant 2$. The results for high Z are then likely to be too small by a factor of about 2 in the neighbourhood of the peak.

The Coulomb-Born approximation is better than the Born, and has been extensively applied, but in the case of $Z = 2$ is significantly in error. The normalized cross sections depend on Z because of the focussing of the nucleus, which is partially screened by the bound electron when $Z \neq 1$, and almost totally unscreened for high Z. The screening is proportional to $(1 - Z^{-1})$. We seek a simple Coulomb focussing factor which depends on Z only through this quantity, and which gives the correct experimental cross section for ionization of H and He^+.

The recommended cross sections are:

$$\tilde{\sigma}_{RZ}(\tilde{E}) = \left[1 + \frac{2.3}{(1 - Z^{-1})^{-2} + 2(\tilde{E} - 1)^2} \right] \tilde{\sigma}_{R(Z=1)} (\tilde{E}) \qquad \ldots (15)$$

Ionization, any Z, any state.

The recommended normalized cross sections for ionization from the ground state when $Z = 1, 2, 5, \infty$ appear in Fig. 1 and are compared with the experimental results of Dolder, Harrison and Thonemann for $Z = 2$.

We recommend the use of the same factor for ionization of any state, so that cross sections for hydrogen may be converted directly to cross sections for any hydrogenic ion.

For high Z the Coulomb-Born-Oppenheimer (C.B.O.) approximation is preferable to our empirical method, but the C.B.O. results of Rudge and Burgess (1963) are suspect following the work on He^+ of Taylor and Burke (1964).

EXCITATION FROM THE GROUND LEVEL OF HYDROGEN

In this and the next section we consider cross sections between levels, without analysing them into the contributions from the individual states of those levels. For most transitions of importance the level transitions are dominated by dipole interactions.

Contributions from other types of interaction are small and difficult to estimate.

This is also true experimentally. The cross sections for excitation are based on the 1s - 2p excitation cross section of Fite and Brackmann (1958) and Fite et al (1959) with a small correction for the 1s - 2s cross section of Stebbings et al (1960) and of Lichten and Schulz (1959).

The interpretation of the experiments is not simple, and is discussed by Seaton (1962a). No convincing theoretical check on these cross sections is available in the neighbourhood of the maximum, but no theory contradicts them. We use them as a basis for the cross section for excitation of the 2 quantum level below 200 eV and above an incident electron energy of a few electron volts above threshold. It has been shown theoretically by Damburg and Gailitis that the cross section is finite at threshold; and this is partially confirmed by the experiment of Chamberlain, Smith and Heddle (1964).

We suppose that the value at threshold is the same proportion of the maximum as in the theory, but that the shape is that of the experiment, which has no absolute scale. This estimate cannot be considered very good. The value at threshold might be in error by a factor of 3, but it is probably better than supposing an incorrect energy behaviour at threshold. The results are summarized graphically in Fig.2. The Bethe approximation is used at higher energies, where it is practically the same as the Born.

The recommended cross section is:

$$\sigma_{R1\to2}(E) = \sigma_{x1\to2}(E) \qquad \text{(Fig.2)} \quad E < 200\text{ eV}$$

$$\sigma_{R1\to2}(E) = \sigma_{B1\to2}(E) \qquad \ldots (16)$$

$$= \frac{2.22}{\tilde{E}}\ (\ln \tilde{E} + 0.69)\,\pi a_0^2 \qquad E > 200\text{ eV}$$

$$\text{Excitation, } Z = 1 \quad \tilde{E} = E/1\text{Ry}.$$

Recent theories show that the detailed energy structure of excitation cross sections below the ionization threshold is much more complicated than crude theories or experiments with poor energy resolution would suggest. However, we do not consider the detailed structure here.

Extensive Born calculations have been made for many other transitions, recently by the St. John's group (Milford and associates) and by Omidvar (1964). McCarroll (1957) obtained $\sigma_{B1\to n'}$ for hydrogen, for $n' = 1$-6. He also obtained a scaling law for high n'. We can improve somewhat on this scaling law by an argument based on classical excitation theory, which suggests that the cross section for excitation into a given small energy interval should be inversely proportional to the cube of the energy difference:

$$\Delta U_n^3 = |U_n - U_1|^3$$
$$= (1 - \frac{1}{n^2})^3 \, Ry^3 \qquad \ldots (17)$$

between the initial and final states. The excitation to a given level n has an additional factor n^{-3} which is the density of levels per unit energy interval.

For comparison of excitation of different levels in the neighbourhood of the threshold we must express the cross sections as functions of the final energy

$$E_n' = E - \Delta U_n \qquad \ldots (18)$$

of the scattered electron. Applying this classical argument to the Born approximation we obtain

$$\sigma_{B1\to n}(E_n') = \frac{\frac{1}{n^3}(1 - \frac{1}{n^2})^{-3} \; \sigma_{B1\to 2}(E_2')}{\frac{1}{2^3}(1 - \frac{1}{2^2})^{-3}}$$
$$= \frac{27}{8(n - \frac{1}{n})^3} \; \sigma_{B1\to 2}(E_2) \qquad \ldots (19)$$

This holds remarkably well, even when comparing with the level n = 2 where the density of states is difficult to define. Comparisons are made in Fig.3. The scaling is similar, but not identical, to that of Seaton (1962a) and van Regemorter (1962) based on the Bethe approximation.

For our recommended cross sections we suppose the same scaling factor to apply to the experimental cross section. In terms of the normalized energy we obtain

$$\sigma_{R,1\to n}(\tilde{E}) = \frac{27}{8(n - n^{-1})^3} \; \sigma_{R1\to 2} \, (\tilde{E} + \frac{1}{n^2} - \frac{1}{4}) \qquad \ldots (20)$$

Excitation, $1 \to n$, $Z = 1$

EXCITATION OF HYDROGEN TO A NEIGHBOURING LEVEL, $n \to n + 1$

Here we recommend the cross sections of Saraph (1964) based on the dipole approximation of Seaton (1962b). This is in some respects a crude approximation, but does take account of the conservation laws, which the Born approximation does not. Neglect of conservation laws grossly overestimates the cross sections in the neighbourhood of the peak probably by a factor of about n. The dipole method has been checked against experiment for the $1 \to 2$ transition, where it is better than the close coupling approximation. It is not clear why this should be so. In this sense the dipole approximation depends on the experiment, since without the check, one would have less confidence in results for higher n.

The cross section is tabulated in a slightly different normalized form than that used here.

$$\sigma(E) = \frac{(5n^2 + 1)^2}{16} \pi a_0^2 X_n^2 \qquad \ldots (21)$$

Excitation $n \rightarrow n + 1$, $Z = 1$

X_n is tabulated as a function of log E in the table which we reproduce as Table 1. The asymptotic form of the cross section for high energies is also given by Saraph.

EXCITATION OF IONS

The effect of Coulomb focussing is less for excitation than for ionization. Owing to the relative weakness of the electron-electron interaction, the Born approximation becomes more reliable. Burke and Smith (1964) and also McCarroll (1964) have obtained the close coupling cross sections for excitation of the $n' = 2$ level of He^+ from the ground level. They do not differ greatly from one of the unpublished Coulomb-Born approximations of Burgess, Hummer and Tully. Indeed the normalized cross section does not differ greatly from the normalized Born cross section for neutral hydrogen. To obtain normalized cross sections for energies greater than 2U, ($\tilde{E} > 2$) we can use the Born approximation for neutral hydrogen.

The energy transfer is not very different for all final states n', and so the same will probably apply to them.

The cross section tends to a finite value at threshold which we take to be, for $n' = 2$:

$$\sigma_{RZ}(\tilde{E}' = 0) = \left[1.1 + 0.6(1 - Z^{-1}) \right] \pi a_0^2 \qquad \ldots (22)$$

Excitation, $1 \rightarrow 2$, $Z > 1$.

These values are consistent with those of Burke and Smith for $Z = 2$, and have the right general behaviour for high Z (Burgess 1961). We shall suppose that the cross section is linear in $\tilde{E}$ between threshold and $\tilde{E} = 2$.

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For Clarification

$$\tilde{\sigma}_{RZ}(\tilde{E}) = (2-\tilde{E}) \left[0.88 + 0.48 \; (1-Z^{-1}) \right] + [0.8 \; \tilde{E} - 0.6] \; \tilde{\sigma}_{B,Z=1}(\tilde{E} = 2) \qquad 0.75 < \tilde{E} < 2$$

$$\tilde{\sigma}_{RZ}(\tilde{E}) = \tilde{\sigma}_{B,Z=1}(\tilde{E}) \qquad \tilde{E} > 2 \qquad \ldots (23a)$$

Excitation $1 \rightarrow 2$, $Z > 1$.

The analytic form of $\tilde{\sigma}_{B,Z=1}(\tilde{E})$ is given by McCarroll (1957). It is

$$\sigma_{B,1\to2}(\tilde{E}) = \left\{F(\tilde{E}^{\frac{1}{2}} + [\tilde{E} - \tfrac{3}{4}]^{\frac{1}{2}}) - F(\tilde{E}^{\frac{1}{2}} - [E - \tfrac{3}{4}]^{\frac{1}{2}})\right\} \pi a_0^2$$

$$F(\zeta) = \frac{2.22}{\tilde{E}} \left[\ln\left(\frac{4\zeta^2}{4\zeta^2+9}\right) + \sum_{S=1}^{4} \frac{1}{S}\left(\frac{9}{4\zeta^2+9}\right)^S\right] \qquad \text{... (23b)}$$

For excitation to higher levels we apply the appropriate scaling law:

$$\tilde{\sigma}_{RZ,1\to n}(\tilde{E}) = \frac{27}{8(n-n^{-1})^3}\, \tilde{\sigma}_{RZ,1\to2}(\tilde{E} + \frac{1}{n^2} - \frac{1}{4}) \qquad \text{... (24)}$$

Excitation, $1 \to n$, $Z > 1$

The scaling laws in Z for $n \to n + 1$ transitions when $n \neq 1$ are more difficult to determine. For large n the dominant contributions to the cross section come from impact parameters large compared with the mean atomic radius, so the effect of Coulomb focussing is unlikely to be significant except for an extremely small energy range just above threshold, which we can safely neglect. The error will probably not be too great even when the initial level is $n = 2$.

However, as the interaction between the electrons is comparatively weak compared to the interaction between either electron and a nucleus of charge Z, the Born approximation satisfies the conservation laws over a much wider range of impact parameters than for $Z = 1$, and the correct normalized cross sections will be reduced from the Born values by a smaller ratio than for the Saraph calculations. We cannot give an estimated cross section, but can only give bounds:

$$\tilde{\sigma}_{R,Z=1}(\tilde{E}) < \tilde{\sigma}_{RZ}(\tilde{E}) < \tilde{\sigma}_{B,Z=1}(\tilde{E}) \qquad \text{... (25)}$$

Excitation, $n \to n + 1$, $n > 1$, $Z > 1$, except just above threshold.

For high Z, say $Z > 4$ the scaled Born cross sections are probably to be preferred. Some have been obtained by Milford and collaborators (See McDowell, M.R.C., ed. Atomic Collision Processes. p.1081.

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TABLE 1

Values of X_n given by Saraph (1964). The cross sections for $n \rightarrow n + 1$ transitions with Z = 1 follow from equation (21). (E in eV)

log E \ n	1	2	3	4	6	8
-0.8					1.12	1.47
-0.6					1.34	1.67
-0.4				0.850	1.55	1.82
-0.2				1.28	1.70	1.93
0.0			1.11	1.48	1.80	1.98
0.2			1.36	1.60	1.84	1.97
0.4		0.956	1.49	1.65	1.81	1.91
0.6		1.22	1.54	1.62	1.73	1.79
0.8		1.28	1.43	1.48	1.56	1.59
1.0		1.23	1.28	1.29	1.32	1.35
1.2	0.529	1.12	1.12	1.12	1.12	1.13
1.4	0.640	0.985	0.981	0.950	0.944	0.948
1.6	0.650	0.852	0.820	0.802	0.991	0.789
1.8	0.611	0.727	0.691	0.672	0.655	0.653
2.0	0.555	0.616	0.580	0.561		
2.2	0.483	0.516	0.483	0.465		

log E \ n	10	15	20	25	30	40
-2.6					0.990	1.31
-2.4				1.01	1.21	1.54
-2.2				1.23	1.44	1.79
-2.0			1.21	1.46	1.68	2.05
-1.8		1.08	1.44	1.70	1.92	2.32
-1.6		1.33	1.66	1.93	2.16	2.59
-1.4	1.03	1.55	1.88	2.16	2.41	2.86
-1.2	1.29	1.77	2.10	2.38	2.64	3.11
-1.0	1.52	1.96	2.29	2.57	2.84	3.33
-0.8	1.72	2.13	2.47	2.74	3.02	3.45
-0.6	1.88	2.28	2.60	2.88	3.14	3.58
-0.4	2.01	2.37	2.68	2.94	3.17	3.57
-0.2	2.09	2.42	2.69	2.92	3.13	3.46
0.0	2.12	2.40	2.64	2.81	2.99	3.30
0.2	2.09	2.31	2.50	2.69	2.82	2.99
0.4	1.99	2.20	2.34	2.44	2.52	2.89
0.6	1.89	2.00	2.08	2.15	2.20	2.29

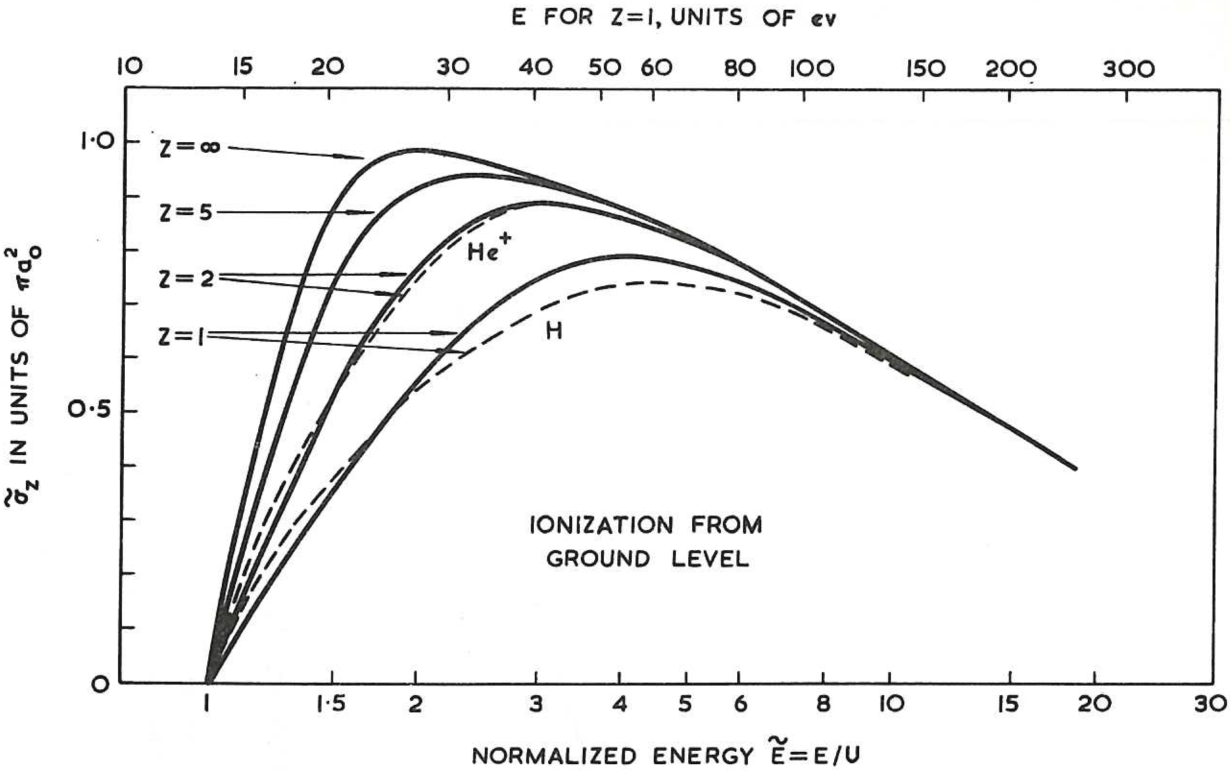

Fig. 1 (CLM-P87)

Continuous curves: recommended normalized cross sections for ionization from the ground level for nuclear charge Z = 1, 2, 5, ∞. Broken curves: experimental results of Boyd and Boksenberg (1959) for H and of Dolder, Harrison and Thonemann (1961) for He^+, where these differ from the recommended cross sections

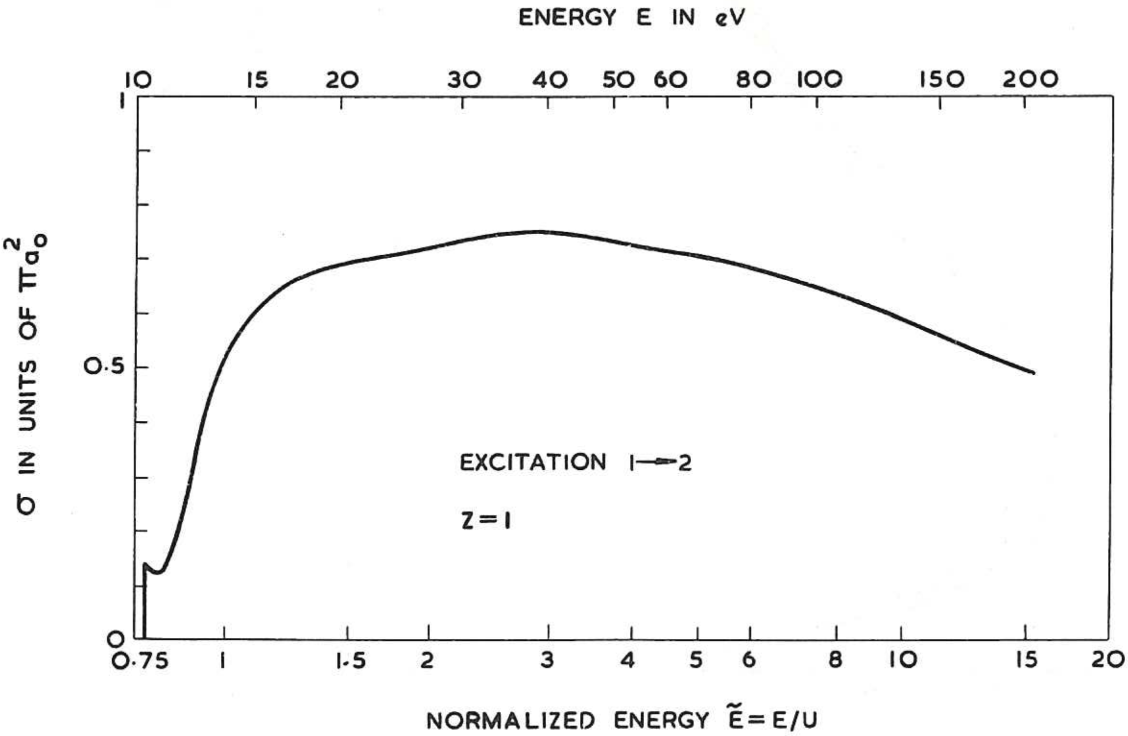

Fig. 2 (CLM-P87)

Recommended cross section for the excitation of the level n = 2 of H based on a combination of experiment and theory (see text)

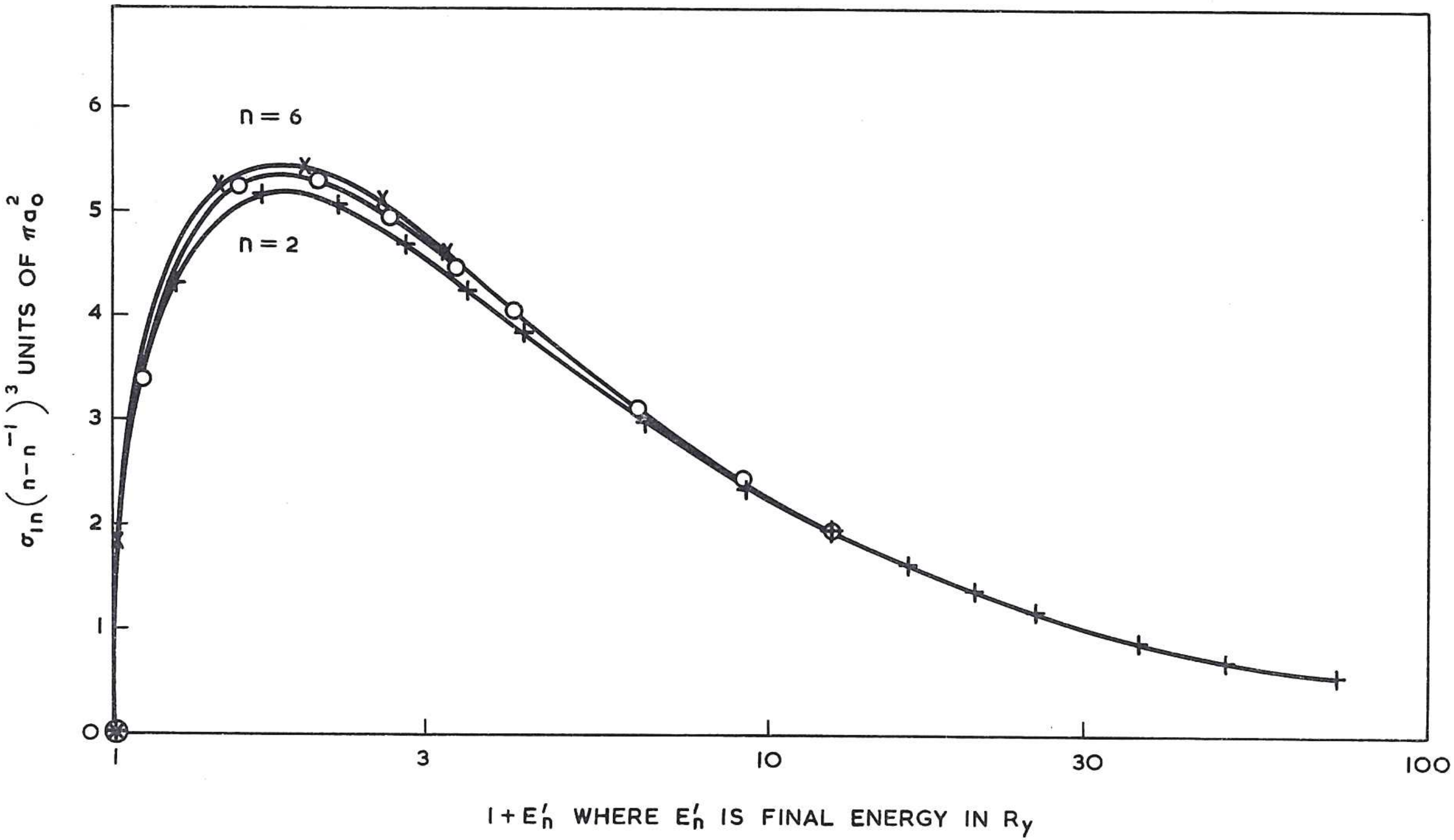

Fig. 3 (CLM-P87)

Graphs of $(n-n^{-1})^3\ \sigma_{B1\to n}(E_n')$ from the Born cross sections of McCarroll (1957) for n = 2, n = 3 and n = 6. These would be the same if equation (19) were exact