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Cross-sections for ionization of positive ions by electron impact

A. Burgess and H. P. Summers *Department of Applied Mathematics and Theoretical Physics, University of Cambridge CB3 9EW*
Deirdre M. Cochrane| *The Cottage, Rubble Pit Lane, Blewbury, Oxfordshire*
R. W. P. McWhirter *Astrophysics Research Division, Appleton Laboratory, Abingdon OX14 3DB*

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Summary. Simple methods of evaluating ionization rate coefficients which have been used in various ionization-balance calculations are compared with values measured in the laboratory. Laboratory measurements are by the crossed-beams method and by plasma spectroscopy, and it is shown that on average both kinds of experiments favour the Exchange Classical Impact Parameter (ECIP) method of calculating ionization rate coefficients although it is not clear why this should be so. This evidence supports Summers' (1974) ionization balance calculations which are based on ECIP ionization cross-sections.

It is also shown that on average the Coulomb–Born calculations, for the small sample considered, are in no better agreement with laboratory measurements near threshold than those by the simpler methods.

1 Introduction

The interpretation of the vacuum ultra-violet spectrum of the outer atmosphere of the Sun and other astronomical objects often involves a calculation of the steady-state ionization balance between the population densities of the highly ionized ions from which the spectra originate. A number of these ionization balance calculations have been done taking account variously of the following processes:

(a) ionization by electron collision including autoionization;
(b) radiative recombination;
(c) dielectronic recombination;
(d) collisional–radiative processes.

Authors who have carried out these calculations are Jordan (1969, 1970), Burgess & Summers (1969), Beigman, Vainshtein & Urnov (1971), Summers (1972, 1974), Nussbaumer & Storey (1975), Jacobs *et al.* (1976). In this paper one of the constituent processes included in all the calculations is considered – namely ionization by electron collision.

Because in the ionization-balance calculations large numbers of different ions have been treated, relatively simple and therefore approximate methods of calculating the coefficients have in general been adopted. For the ionization rate coefficients the semi-empirical formula (SEF) given by Seaton (1964) following a procedure introduced by Elwert (1952), and the exchange classical impact parameter method (ECIP) described by Burgess (1964), have been adopted (Beigman *et al.* 1971 used a simplified Coulomb–Born approximation.) Thus the central questions to which this paper addresses itself are: 'How do these simple methods compare with the best experimental data?' and 'How well do more sophisticated theoretical calculations, e.g. the Coulomb–Born calculations of Moores (1972), reproduce the experimental values?' Presnyakov (1975) has studied the relation between Coulomb–Born cross-sections and Seaton's formula. He finds that the latter should be considered a lower limit to the proper value which he identifies with the Coulomb–Born results. It will be seen that the conclusions of the present paper are somewhat different.

Measurements of ionization cross-sections (or the related rate coefficient equal to the Maxwellian average of the cross-section times the electron velocity), have been done by two methods:

(a) Crossed-beams method reviewed by Dolder (1969).
(b) Plasma spectroscopy method reviewed by Kunze (1972).

The first method, (a) is capable of good accuracy (±10 per cent) but has been limited to ions of charge one and two. Measurements of cross-sections have been made with good energy resolution over a wide range of electron energies. Recent developments in ion sources promise a valuable extension of this work to ions of higher charge. With the second method, (b) it is possible to measure rate coefficients for ions of higher charge but with less accuracy and for a limited energy range with the rather poor energy resolution determined by the spread of the Maxwellian velocity distribution of the plasma electrons. However, it should be noted in favour of this method that the conditions of ionization resemble more closely the conditions in the solar atmosphere.

It has been pointed out by Goldberg, Dupree & Allen (1965) that autoionization can make substantial contributions to the total ionization rate. The additional process of collisional ionization of metastable ions increases the total rate of ionization but this has been ignored in the ionization balance calculations. For the present purposes attention is confined to the direct ionization of ions in their ground configurations by electron impact including, where appropriate, the contributions of inner shell ionization and autoionization.

Inspection of the results of the ionization balance calculations shows that the ionization potential of the most populous ion in a given plasma is between three and ten times the mean energy of the free electrons of the plasma. This means that the calculation is dominated by the magnitude of the cross-sections near threshold (electron energies up to twice the threshold energy and therefore lying towards the high-energy tail of the Maxwellian) and for this reason attention in this paper is confined to this limited energy range. For the same reason Seaton's formula was designed to be applicable only in this threshold energy range. Strictly speaking, none of the formulae we discuss has the correct (non-linear) threshold behaviour (Wannier 1953) but the effects of this are very small in comparison with the accuracies with which we are concerned here. However, it turns out that data are required outside this energy range for some laboratory plasmas and that the use of SEF outside its range of validity introduces significant errors for some ions of very high charge ($> \sim 25$). In these circumstances it is better to use an empirical formula due to Lotz (1967) since for ions of charge greater than 3 it gives almost the same threshold values (for electron energies less than twice threshold, $0.87 < \text{Lotz/SEF} < 1.26$), while for energies much greater than threshold it is a better representation of true cross-sections. For ions of charge less than 4, Lotz' formula includes additional parameters that have effects apparent in some of the data presented in this paper.

The ECIP results were obtained using the procedure of Burgess (1964) (see also Burgess & Percival 1968, p. 124) in the simplified form detailed in Burgess & Summers (1976) (with insertion of the usual factor ζ to take account of the number of equivalent electrons). For the bound–free oscillator strengths (df/dE) hydrogenic ion expressions were used (with principal quantum number n replaced by effective principal quantum number ν, and the bound–free Kramers–Gaunt factor set to unity). Similarly the mean atomic radius was taken as $\bar{r} = (5\nu^2 + 1)/4z$. These two approximations were made for two main reasons.

First, the near threshold ionization cross-section is insensitive to df/dE and $\bar{r}$, the IP contribution being relatively small. This is fortunate, as accurate values of df/dE are not easily obtainable for all of the cases we wish to consider here. It might be thought that an expression for $\bar{r}$ which depends on orbital angular momentum quantum number, such as $\bar{r} = (3\nu^2 - l(l+1))/2z$, would be preferable, but this is certainly not the case for the ground state of many of the ions considered here (e.g. for some $2p^6$ ions this expression would give negative values of $\bar{r}$). The sensitivity to $\bar{r}$ was tested by comparing with ECIP results obtained using the first order Coulomb approximation expression $\bar{r} = \nu(\nu + \frac{1}{2})/z$ (which does give quite good $\bar{r}$ values for $2p^6$ ions); in all cases the two sets of ECIP results differ by less than 2 per cent near threshold.

Second, this is the same procedure as adopted in ionization-balance calculations under discussion (Burgess & Summers 1969, 1976; Summers 1972, 1974). In this connection it is important to repeat (see, e.g. p. 1014 of the first of those papers) that those calculations were primarily calculations of recombination coefficients, with less attention paid to the ionization coefficients. The two coefficients are separable to a very good approximation so that the ionization balance curves may easily be modified to take into account different rates of ground-state ionization. Thus the reasons for adopting ECIP in those calculations were (i) the formula must be reasonably simple (since many excited levels may be involved); (ii) the formula must have the correct behaviour for highly excited states (i.e. for incident electron energies $\gg$ threshold) which are the ones of main importance for recombination; (iii) the formula should give fairly reasonable (and easily correctable) results for ground state ionization. It should be clear that for ground state ionization ECIP has no prior claim to superiority over other ionization formulae.

The ECIP formula was used in a similar straightforward manner to calculate direct ionization from inner shells, although these contributions are mostly not of much importance for the considerations of this paper, as the inner-shell direct ionization threshold energy is usually appreciably higher than that of the outer shell. For some of the ions considered here there are important contributions arising from inner-shell excitations followed by auto-ionization. They fall into two reasonably distinct categories: (i) those in which the lowest configuration obtainable by excitation of an inner-shell electron is clearly above the outer-shell ionization threshold (e.g. Ca^+ $3p^6 4s \rightarrow 3p^5 3d 4s$); (ii) those in which it is well below (e.g. C^+ $2s^2 2p \rightarrow 2s 2p^2$). Intermediate cases may of course occur but they are rather rare, and fortunately do not arise here. Case (i) leads to a finite jump (or series of jumps) in the cross-section which may be calculated easily with ECIP if the relevant oscillator strengths are known. However, since these occur well above threshold and we are interested in the near-threshold behaviour, we have not included those contributions here. In case (ii) the auto-ionization states must (by definition) lie well above the lowest excited inner-shell electron state, so that they belong to configurations of larger principal quantum number. As a result there are many such states near to the outer-shell ionization threshold, and they remain closely packed up to the inner-shell direct ionization threshold (e.g. in C^+, $2s\,2p\,3d$, $2s\,2p\,4s$, etc, states lie densely between the $2p$ and the $2s$ ionization thresholds). Also, almost all of the states arising from these configurations will be autoionizing (provided they lie in the continuum) and the resulting closely spaced small finite jumps in the ionization cross-section will usually be indistinguishable (both for cross-beam cross-section measurements and for ionization rate coefficient calculations in plasmas) from a continuous curve rising from zero at the outer shell ionization threshold. Thus, the effective threshold for ionization from the inner shell is lowered to that of the outer shell and, to a good approximation, one may take into account all inner-shell contributions (both autoionization and direct ionization) by increasing ζ by the number of inner-shell electrons concerned (e.g. for C^+ the ionization potential is 24.4 eV with $\zeta = 3$ instead of 1). Note that the correspondence principle leads to smoothness of the total cross-section curve at the inner-shell threshold (taken for simplicity as the mean of the thresholds for the $1s^2\,2s\,2p\,{}^3P$ and ${}^1P$ final states in the case of C^+). This procedure may be applied both with ECIP and Seaton's formula and we have adopted it for all case (ii) ions.

Much of the remainder of this paper consists of a comparison of the experimental results with the various predictions mentioned above together with a discussion of the implications of this comparison for the ionization-balance calculations. The effect on the ionization balance of changing the ionization rate coefficients by, say, a factor 2 is discussed and found to be relatively small at low temperatures ($T < 10^5$ K) but at higher temperatures it can be substantial.

2 Review of the results of measurements of ionization cross-sections by the crossed-beams method

A comprehensive review of the earlier measurements by this method was prepared by Dolder (1969). The main emphasis in his review is on energies much greater than threshold where agreement with the theoretical Coulomb–Born (and even Born) approximation is good. Although Dolder does remark that threshold values are in poor agreement with theory, the general impression given by the review is that when the whole range is considered there is no important discrepancy. In the present review we start by recognizing that the threshold values of the cross-sections dominate in the ionization balance calculations (electron energies up to twice threshold). When experiment and theory are compared in this range a different and less satisfactory conclusion is reached. In this review we concentrate on the more recent measurements where near-threshold experimental errors are smaller (less than ±15 per cent); this also limits the comparisons to a manageable number. Before discussing the individual measurements in detail it may be helpful to present a brief description of the experimental method. A more detailed description, especially covering the causes of experimental uncertainty, is given by Dolder (1969).

Ions from an ion source are accelerated and passed into an ion selector which may be either a magnetic or an electro-static field. The selected ions then pass into the collision region where they intersect an electron beam. The resulting ion beam enters an analyser which again may be magnetic or electro-static and which separates the products of the collisions from the original beam. Suitably placed ion collectors are then used to measure the absolute beam fluxes. In order to determine the absolute cross-section for the reaction being studied, it is necessary to measure the so-called form-factors for both colliding beams. This is done by moving shutters with slots across each beam in turn and measuring the transmitted flux as a function of slot position. Spurious results due to background gas in the apparatus are corrected for by pulsing the beams in various combinations of phases. In analysing the results care has to be taken to account for the proportion of incident ions in excited or metastable states. The reported measurements that have been chosen for inclusion in this review are now discussed individually. The basis of choice is that they should be relatively recent (since 1968) and that the target ion should have charge of +1 or greater. There are 11 papers from three groups of workers reporting measurements on 16 ions.

Peart & Dolder (1968) measured the cross-sections for ionization of Na^+ to Na^{2+} and K^+ to K^{2+}. In the range of interest for the present review the authors estimate the accuracy of their results to be ± 6 per cent. They used a thermionic ion source that produced the ions in their ground levels. The contribution of autoionization for those ions with complete outer shells is probably negligible. Thus the dominant process is direct ionization including small contributions due to the inner $2s^2$ or $3s^2$ shells from the ions in their ground configurations.

The experimental results for Na^+ are reproduced in Fig. 1 where the cross-section is plotted as a function of $\log(E/\chi)$ where E is the incident electron energy and χ is the ionization potential of the outermost shell ($2p^6$ in this case). This method of plotting emphasizes the threshold behaviour of the cross-sections. Results at high electron energy are excluded. Attention should be concentrated on the first quarter of the plot where electron energies are less than twice threshold ($\log E/\chi \leqslant 0.3$). This is true for all similar plots in this review paper.

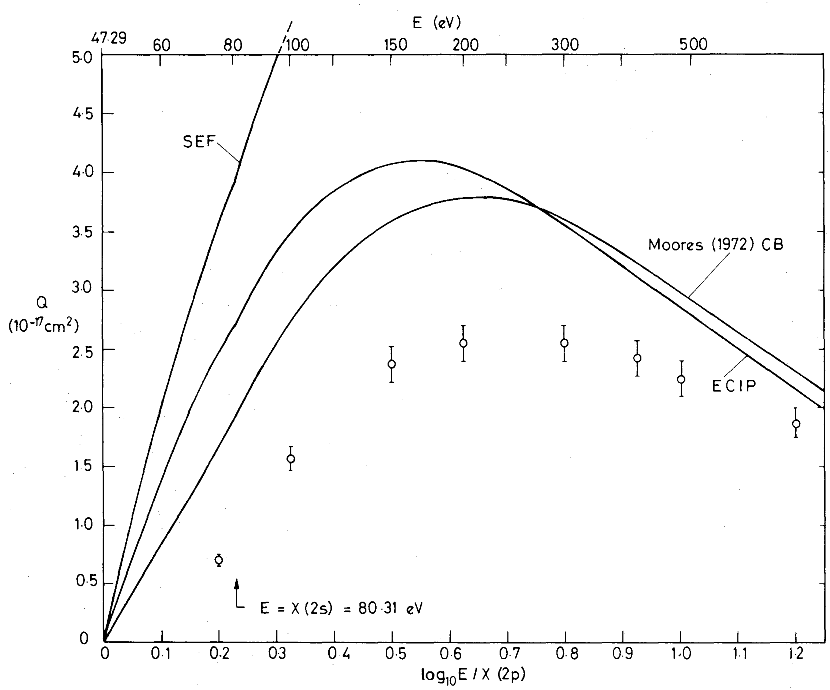

Figure 1. The ionization cross-section for Na^+ in its ground configuration, $2s^2\,2p^6$: $Na^+ + e \rightarrow Na^{2+} + 2e$. The experimental points are those of Peart & Dolder (1968).

For comparison with the experimental data the values calculated using Seaton's (1964) formula and the ECIP approximation are shown. In both cases inner-shell ionization from the $2s^2$ shell is included. Finally the Coulomb–Born values of Moores (1972) are also shown but are discussed later.

Comparison of the experimental values with the SEF and ECIP results are presented in Table 1. Note that only two experimental measurements fall within our approximate range of interest. In a similar manner the K^+ data was plotted except that no Coulomb–Born data appears to be available. Again there were only two measurements within the approximate range of interest and these are compared with the predicted values in Table 2.

Table 1. Na^+.

E/χ	SEF/expt	ECIP/expt	C–B/expt
1.59	5.04	3.54	2.39
2.11	3.33	2.21	1.73

Table 2. K^+.

E/χ	SEF/expt	ECIP/expt	C–B/expt
1.57	1.00	0.53	NA
2.36	1.35	0.72	NA

Martin, Peart & Dolder (1968) have reported a measurement of the cross-section for ionization of Mg^+ to Mg^{2+} with a claimed experimental accuracy of ±10 per cent. They made three measurements in our range of interest. Their results are displayed in Fig. 2 along with the SEF and ECIP values. The Coulomb–Born results of Moores & Nussbaumer (1970) are also shown as well as Lotz' (1967) prediction. This ion does not have any metastable levels which can influence the experimental results. Bely (1968) predicted a large contribution due to autoionization at energy thresholds of $E/\chi(3s) = 3.8$ and 6.7. Moores & Nussbaumer (1970) find a smaller contribution (see Fig. 2) but in any case the thresholds are outside our range of interest. Comparison of the predicted cross-sections with experiment is made in Table 3. Peart & Dolder (1968) measured the cross-sections for ionization of Li^+ and Ba^+ but measurements for Ba^+ have been repeated by Peart, Stevenson & Dolder (1973) more recently and will be considered later in their chronological order.

For H-like and He-like ions the SEF and ECIP values are closely equal and also agree approximately with the Coulomb–Born values. This is apparent for He-like Li^+ in Table 4. Only one experimental value for Li^+ falls within the specified range although two values have been included in Table 4. The experimental accuracies for the two points are given as 15 and 6 per cent respectively.

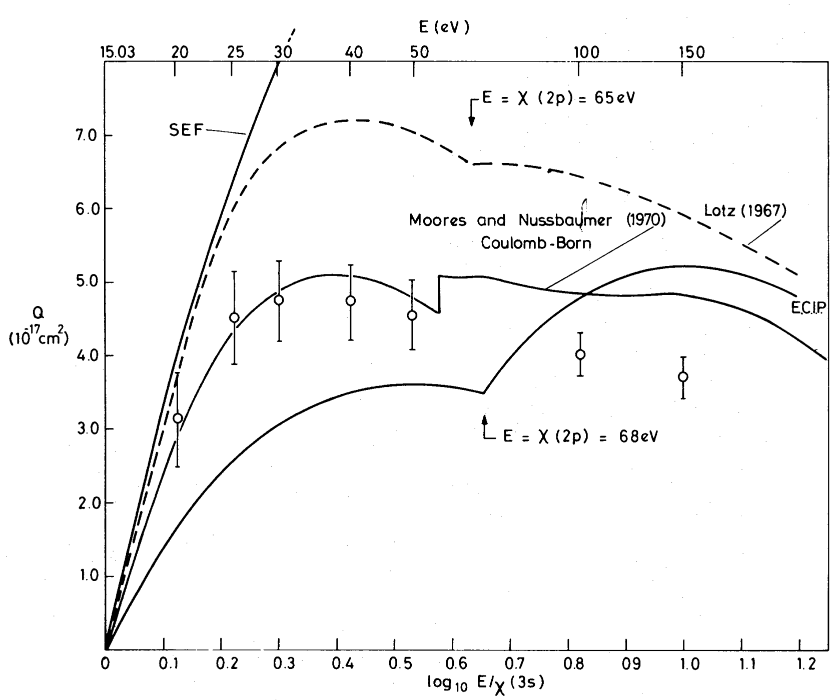

Figure 2. The ionization cross-section for Mg^+ in its ground configuration, $2p^6\,3s^1$: $Mg^+ + e \rightarrow Mg^{2+} + 2e$. The experimental points are those of Martin, Peart & Dolder (1968).

Table 3. Mg^+.

E/χ	SEF/expt	ECIP/expt	C–B/expt
1.33	1.25	0.53	0.91
1.67	1.42	0.57	0.96
2.00	1.66	0.64	1.03

Table 4. Li^+.

E/χ	SEF/expt	ECIP/expt	C–B/expt
1.32	1.89	1.89	1.41
2.64	2.00	1.56	1.44

Peart, Martin & Dolder (1969) measured the cross-section for the ionization of Mg^{2+} to Mg^{3+} and these values are compared with the predictions by the SEF, ECIP and Moores. Three points lie within the range, measured to an accuracy of 5, 2 and 6 per cent respectively. These are compared in Table 5 with the SEF and ECIP values in which the inner-shell ionization from the 2*s* shell is taken into account.

Peart, Walton & Dolder (1969) report measurements for the ionization of He^+ (also Li^+ but only for high electron energies). These are compared in Fig. 3 with values calculated by the SEF and ECIP methods as well as various Coulomb–Born calculations discussed later. Table 6 gives the usual ratios.

Table 5. Mg^{2+}.

E/χ	SEF/expt	ECIP/expt	C–B/expt
1.26	2.56	1.67	1.93
1.50	1.64	1.09	1.29
1.86	1.89	1.18	1.39

Table 6. He^+.

E/χ	SEF/expt	ECIP/expt	C–B/expt
1.25	1.6	1.27	1.47
1.53	1.51	1.19	1.33
1.80	1.51	1.12	1.31

Aitken & Harrison (1971) measured the cross-sections for ionization of O^+ to O^{2+} and O^{2+} to O^{3+}. In the prediction of the theoretical values the inner-shell ionization from the $2s^2$ shell has been included in both cases and the effect of autoionization has also been included as described in Section 1. The tabulated results show the comparisons of values with and without the effect of autoionization. For both the ionization of O^+ to O^{2+} and O^{2+} to O^{3+} a considerable number of experimental points are available. The additional effect of autoionization can be seen to increase the discrepancy between the SEF values and experimental values, whereas the ECIP values are raised from just below the experimental values to just above them.

For O^{2+} to O^{3+} the first four values in Table 8 have errors estimated by Aitken & Harrison to be greater than ±15 per cent and have therefore been excluded from the averaging procedure discussed later.

Aitken, Harrison & Rundel (1971) also obtained experimental values for N^{2+} to N^{3+} and C^+ to C^{2+}. The experimental data in the case of C^+ has been modified to allow for the 1-eV

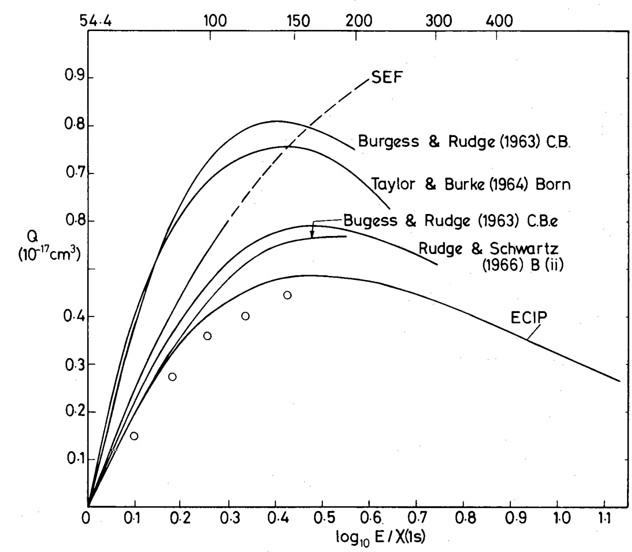

Figure 3. The ionization cross-section for He^+ in its ground configuration, $1s^1$: $He^+ + e \rightarrow He^{2+} + 2e$. The experimental points are those of Peart, Walton & Dolder (1969).

Table 7. O^+.

E/χ	Without autoionization		With autoionization		C–B/expt
	SEF/expt	ECIP/expt	SEF/expt	ECIP/expt	
1.08	1.10	0.62	1.83	1.03	0.79
1.14	1.39	0.80	2.32	1.33	1.00
1.22	1.47	0.84	2.46	1.40	1.07
1.37	1.59	0.82	2.25	1.27	1.07
1.51	1.67	0.87	2.20	1.27	1.13
1.65	1.74	0.92	2.18	1.26	1.14
1.93	1.79	0.93	2.20	1.20	1.18

Table 8. O^{2+}.

E/χ	Without autoionization		With autoionization		C–B/expt
	SEF/expt	ECIP/expt	SEF/expt	ECIP/expt	
1.06	0.55	0.33	1.11	0.66	
1.13	0.54	0.31	1.07	0.62	
1.17	0.48	0.26	0.97	0.53	
1.24	0.72	0.35	1.15	0.62	
1.42	0.87	0.41	1.20	0.62	0.85
1.55	0.87	0.43	1.17	0.63	0.87
1.73	1.02	0.50	1.29	0.66	0.88

reduction in ionization potential discussed by the authors. In both cases, the theoretical calculations compared with them have taken into account the inner-shell ionization, and Tables 10 and 11 show the comparative ratios with and without the effect of autoionization. The N^{2+} results are plotted in Fig. 4. A good selection of experimental points are in the range for both ions, and the results slightly favour the SEF.

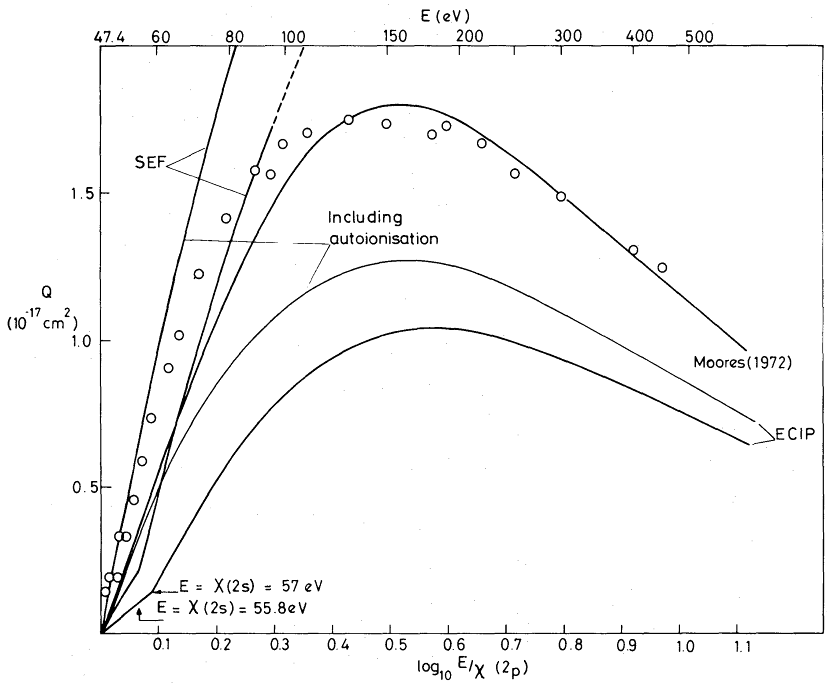

Figure 4. The ionization cross-section for N^{2+} in its ground configuration, $2s^2 2p^1$: $N^{2+} + e \rightarrow N^{3+} + 2e$. The experimental points are those of Aitken, Harrison & Rundel (1971).

Table 9. N^{2+}.

E/χ	Without autoionization		With autoionization		C–B/expt
	SEF/expt	ECIP/expt	SEF/expt	ECIP/expt	
1.06	0.52	0.24	1.57	0.71	0.82
1.08	0.33	0.16	0.99	0.47	0.55
1.10	0.47	0.22	1.40	0.67	0.78
1.15	0.43	0.21	1.28	0.64	0.71
1.19	0.44	0.21	1.31	0.64	0.70
1.23	0.55	0.20	1.20	0.61	0.68
1.31	0.67	0.27	1.25	0.64	0.71
1.40	0.77	0.32	1.28	0.64	0.75
1.48	0.81	0.35	1.27	0.63	0.74
1.65	0.91	0.42	1.35	0.64	0.80
1.86	1.00	0.46	1.36	0.65	0.85
1.97	1.09	0.49	1.45	0.69	0.92

Table 10. C^{+}.

E/χ	Without autoionization		With autoionization		C–B/expt
	SEF/expt	ECIP/expt	SEF/expt	ECIP/expt	
1.03	0.36	0.21	1.07	0.62	0.38
1.12	0.59	0.29	1.76	0.88	0.63
1.20	0.61	0.30	1.82	0.89	0.64
1.40	0.78	0.34	1.69	0.83	0.67
1.61	1.00	0.45	1.78	0.85	0.77

Table 11. Ba^+.

E/χ	SEF/expt	ECIP/expt	
1.18	1.10	0.95	
1.28	0.75	0.59	
1.30	1.24	0.94	(Feeney *et al.*)
1.38	1.01	0.68	
1.48	0.96	0.59	
1.55	0.65	0.37	(Feeney *et al.*)
1.58	0.91	0.50	

The Ba^+ measurements of Peart *et al.* (1973) produced five points in range and to these are added two results by Feeney, Hooper & Elford (1972). Inner-shell ionization has a marked effect but is outside the range, as is the effect of autoionization as calculated by Bely, Schwartz & Val (1971).

Peart & Dolder (1975) published measurements for the ionization cross sections for Rb^+, Cs^+, Ca^+ and Sr^+. For Rb^+ and Cs^+ three and four results respectively are in range and there is no experimental evidence of autoionization.

Table 12. Rb^+.

E/χ	SEF/expt	ECIP/expt
1.38	1.64	0.86
1.56	1.11	0.58
1.75	1.0	0.50

Table 13. Cs^+.

E/χ	SEF/expt	ECIP/expt
1.32	0.92	0.45
1.52	0.90	0.45
1.71	1.03	0.51
1.91	1.07	0.52

For Ca^+ and Sr^+ a good selection of experimental results is available. The effect of inner-shell ionization falls outside the range but the experimental results show a marked effect of autoionization at 27.5 eV for Ca^+ and a slightly less dramatic effect between 22 and 30 eV for Sr^+.

Table 14. Ca^+.

E/χ	SEF/expt	ECIP/expt
1.05	1.96	0.71
1.13	2.13	0.85
1.22	1.95	0.78
1.30	2.00	0.81
1.39	1.99	0.79
1.55	2.07	0.82
1.64	2.25	0.88
1.72	2.11	0.81
1.81	2.31	0.87

Table 15. Sr^+.

E/χ	SEF/expt	ECIP/expt
1.11	2.55	1.09
1.20	2.04	0.86
1.29	1.97	0.79
1.47	2.50	0.97
1.56	2.00	0.77
1.65	2.32	0.90
1.65	2.04	0.79
1.83	1.97	0.74

Measurements of the ionization cross-section of Tl^+ have been made by Divine *et al.* (1976). In using the SEF and ECIP methods for this ion we take account of inner-shell ionization and autoionization by grouping all 12 of the outermost electrons together ($5d^{10}6s^2$, i.e. $\zeta = 12$) and use the ionization potential appropriate to the $6s^2$ electron (see Section 1). Table 16 compares the ratios of the results in the usual way.

Table 16. Tl^+.

E/χ	SEF/expt	ECIP/expt
1.10	4.18	1.84
1.22	3.88	1.73
1.47	3.85	1.72
1.71	4.17	1.84
1.96	3.68	1.48

The results of the comparisons made above are presented in Table 17 where the averaged ratios for each ion are shown. Identical values have been inserted in columns labelled 'with' and 'without autoionization' in those cases where it does not contribute (see Section 1). These values are now averaged to give Table 18, with the standard deviations in brackets. This method of averaging by taking arithmetic means of ratios can be criticized if the

Table 17.

Ion	Without autoionization		With autoionization	
	SEF/expt	ECIP/expt	SEF/expt	ECIP/expt
Na^+	4.19	2.88	4.19	2.88
K^+	1.18	0.63	1.18	0.63
Mg^+	1.44	0.58	1.44	0.58
Li^+	1.89	1.89	1.89	1.89
Mg^{2+}	2.03	1.30	2.03	1.30
He^+	1.54	1.19	1.54	1.19
O^+	1.54	0.83	2.21	1.25
O^{2+}	0.92	0.45	1.22	0.64
N^{2+}	0.67	0.30	1.31	0.64
C^+	0.67	0.32	1.62	0.81
Ba^+	0.95	0.66	0.95	0.66
Rb^+	1.25	0.65	1.25	0.65
Cs^+	0.98	0.48	0.98	0.48
Ca^+	2.09	0.81	2.09	0.81
Sr^+	2.17	0.86	2.17	0.86
Tl^+	3.95	1.72	3.95	1.72

Table 18.

	Without autoionization	With autoionization
Averaged ratio SEF/expt	1.72 (± 61 per cent)	1.88 (± 51 per cent)
Averaged ratio ECIP/expt	0.97 (± 71 per cent)	1.06 (± 60 per cent)

denominators in the ratios are small as may happen here near threshold. To check on this we also calculated the ratio of the arithmetic means of the cross-sections and found a difference of less than 5 per cent in the final results.

3 Review of results of measurements by the Plasma Spectroscopy method

Kunze (1972) has reviewed the available results of measurements by this method up to 1972, and more recently Datla, Nugent & Griem (1976) have revised the analysis of the measurements by the University of Maryland group. The conclusions of these authors is broadly in agreement with those presented here. However, before discussing the measurements a brief description of the experimental method may be helpful.

The method depends on making time-resolved measurements of the intensities of spectral lines (in arbitrary units) of the ions of interest as emitted from a pulsed laboratory plasma – usually from a device known as a theta pinch. These measurements are made with a photomultiplier recording the emission in one spectral line at the focal plane of a vacuum spectrometer. The signal detected in this way, for a low-density plasma, may be shown to be given by the following expression (McWhirter 1975)

$$I = k_1 n_e n_i T^{-1/2} \exp(-\chi/kT) L,$$

where k_1 is a constant depending on: (a) the spectral sensitivity; (b) the geometrical arrangement; and (c) the atomic constants of the transition detected; n_e is the electron density at the instant of observation; n_i is the population density of the relevant ion in its ground or metastable level at the instant of observation; T is the electron temperature at the instant of observation; χ is the excitation potential of the upper level from the ground or metastable level and L is the physical depth of the plasma as viewed by the spectrometer.

Since I is in arbitrary units the only requirements of the measurement system are spectral purity and linearity of response. The determination of the plasma parameters (n_e, T and L) are by a number of methods described below but generally requiring a measurement of T by the laser-scattering technique. The population density (n_i) of the ion being studied is determined by solving the time-dependent ionization equation (McWhirter 1975)

$$\frac{dn_i}{dt} = n_e n_{i-1} S_{i-1} - n_e n_i S_i - n_e n_i \alpha_i + n_e n_{i+1} \alpha_{i+1},$$

where S and α are ionization and recombination rate coefficients respectively. S is defined as the product of the ionization cross-section and the electron velocity averaged over a Maxwellian distribution. The recombination coefficient α has negligible effect on the solution in the circumstances of these measurements and need not be discussed here. It is the solution of this time-dependent ionization equation that predominantly determines the time history of the spectral intensities. The method of analysis is to adjust the values of the ionization rate coefficients until the solution of the equations gives the same time dependence of intensity variation as observed experimentally. Since the plasmas used for these studies are spatially homogeneous to an adequate extent, the equations as given take account of any variation in the plasma dimensions with sufficient accuracy. There is a more complete discussion of possible sources of experimental uncertainty in the paper by Lang (1977, in preparation). Relevant measurements are discussed individually below.

The first report of measurements of ionization rate coefficients by this method is by Hinnov (1966, 1967) who studied neon. In this work the electron temperature of the plasma (produced in a stellarator) was determined by measuring its electrical conductivity and using Spitzer's (1962) relation connecting them. (Hinnov's second paper (1967) corrects an earlier error in applying this method.) This is a less direct way of determining the electron temperature than by laser scattering which had not been sufficiently developed at that time. Another difficulty with this measurement, discussed by Hinnov, was the suspicion that the electron velocity distribution was not Maxwellian.

The results of the measurement are in strong disagreement with all the other measurements discussed in this review, since the experimental ionization rate coefficients are *larger* than the values given by Lotz' or Seaton's formulae. The ratio of the values found by Hinnov to those calculated using Lotz' formula are as follows for the various ions of neon which were present at the temperatures listed.

Ion	Ne^{2+}	Ne^{3+}	Ne^{4+}	Ne^{5+}	Ne^{6+}	Ne^{7+}
Temperature (K)	1.7×10^5	2.3×10^5	3.5×10^5	4.6×10^5	5.8×10^5	7.0×10^5
S(Lotz)/S(expt)	1.0	0.67	0.50	0.33	0.43	1.0

In discussing Hinnov's work in his review Kunze (1972) made an error in relating the measured to the theoretical values which he now acknowledges (private communication).

The next group of five papers are all the work of the University of Maryland group who have reported more results than any other in this field. In the first of these Kunze, Gabriel & Griem (1968) report measurements of the ionization rate coefficient for helium-like C^{4+}. The electron temperature and density were measured by the laser-scattering technique, and in addition the intensity of the continuum was measured as an additional check on the density. The authors estimate their measurement accuracy to be in the range ±25 to ±50 per cent, and their values for the ionization rate coefficient agree with Lotz' and ECIP values to within this accuracy. (For helium-like and hydrogen-like ions Lotz' and ECIP cross-sections are in approximate agreement with each other.)

Kunze (1971) reports measurements of ionization rate coefficients for lithium-like C^{3+}, N^{4+} and O^{5+} and beryllium-like O^{4+} and Ne^{6+}. Again the electron temperature and density were measured by the laser-scattering technique but there is no report of a density check by measuring the continuum intensity. The results of the measurements give values lower than those given by the Lotz formula but, since the analysis is revised in the last paper of this group, the discussion is held over till that paper is considered.

Datla, Kunze & Petrini (1972) using the same method as Kunze (1971) report a measurement for sodium-like Ar^{7+} with similar results also discussed below.

Reporting further work by the same group Datla, Blaha & Kunze (1975) give values of Fe^{7+}, Fe^{8+} and Fe^{9+}. The authors have taken account of the substantial contribution to the cross-section due to inner-shell ionization and find their experimental values to be about half the values based on the Lotz formula. This analysis is also revised in the paper discussed next.

Datla, Nugent & Griem (1976) report a repeat measurement of helium-like C^{4+} and also B^{3+} ionization. This time comparison is made with the theoretical values based on the ECIP approximation (Burgess 1964). These authors have taken the experimental results of the three papers discussed immediately before this and revised the analysis so as to make comparison with the ECIP values. Their results are reproduced in the accompanying table. This table shows that in all cases theory (ECIP) and experiment agree within the estimated experimental accuracy (25–50 per cent).

Table 19.

Ion	kT/χ	S (ECIP) (cm^3/s)	S (Experiment) (cm^3/s)	S (ECIP)/S (Expt)
B^{3+}	0.77	3.0×10^{-10}	$2.4\ (\pm 0.7) \times 10^{-10}$	1.25
C^{4+}	0.55	8.0×10^{-11}	$8.0\ (\pm 2.0) \times 10^{-11}$	1.00
C^{3+}	2.33	1.29×10^{-9}	1.52×10^{-9}	0.85
N^{4+}	2.04	6.7×10^{-10}	6.3×10^{-10}	1.06
O^{5+}	1.45	3.1×10^{-10}	3.5×10^{-10}	0.89
O^{4+}	1.23	7.4×10^{-10}	7.0×10^{-10}	1.06
Ne^{6+}	0.96	2.2×10^{-10}	2.9×10^{-10}	0.76
Ar^{7+}	1.81	3.0×10^{-10}	5.2×10^{-10}	0.58
	1.01	1.7×10^{-10}	2.0×10^{-10}	0.85
Fe^{9+}	0.54	1.5×10^{-10}	1.8×10^{-10}	0.83
Fe^{8+}	0.53	2.1×10^{-10}	2.7×10^{-10}	0.78
Fe^{7+}	0.73	3.5×10^{-10}	3.0×10^{-10}	1.17
		Average value (standard deviation)		0.92 (± 21 per cent)

Some recent work on the ions of neon, namely Ne^{5+}, Ne^{6+} and Ne^{7+}, is reported by Jones, Källne & Thompson (1977) They used laser scattering to measure the electron temperature of their theta-pinch plasma and an interferometric method of determining its electron density. They compare their results with the values obtained using a formula within 10 per cent of Lotz and find ratios of predicted to experimental rate coefficients between 6.7 and 1.4. However, it is not clear from their paper how they have made the comparison in detail. They state that they have not included inner-shell ionization and there is no mention of autoionization nor of ionization from metastable levels. The inclusion of these processes could increase the discrepancy between the experiment and predictions.

Finally Lang (1977) reports some further measurements for neon (Ne^{4+}, Ne^{5+} and Ne^{6+}) using a theta pinch. In this case both temperature and density were measured by laser scattering. His results again show a similar disparity with the rates calculated from Lotz' formula and as reported by other workers. He finds ratios of calculated (Lotz' formula) to experimental rate coefficients of about 4.0.

Thus the conclusion of this part of this review is that, as before, the ECIP approximation is a better representation of the experimental data than Seaton's or Lotz' formula. The only results at variance with this conclusion are the early work of Hinnov (1966, 1967) which should perhaps be discounted since the necessary experimental techniques were not fully developed at that time.

4 The implications for ionization balance calculations

Reference has already been made in the introduction to the various ionization-balance calculations. All of these except Burgess & Summers (1969) and Summers (1974) have made use of Seaton's formula for ionization or methods that give similar values. These exceptions made use of the ECIP method that has been shown above to give values in better agreement on average with the experimental measurements.

It is of interest to enquire how much difference does a change of, say, a factor 2 in the ionization rate coefficients make to the results of the ionization-balance calculation. With the object of studying this the ECIP rate coefficients of Summers' calculation were increased by $\times$ 2 (for neon at $n_e = 10^8\,\text{cm}^{-3}$) and the ionization-balance calculation repeated. The complete details of the other coefficients used in the calculation are given by Summers (1974).

Fig. 5 shows the coefficients (ECIP × 1) that were used in the calculation. The crossing points of corresponding ionization and recombination curves are marked on this diagram and indicate the temperature values at which ions of neighbouring charge have equal population densities in the steady state. The diagram also shows clearly how it is the steepness of the variation of ionization rate with temperature that determines the range of temperature at which a particular ion reaches a particular population density near its peak. It should also be noted how the steepness of these curves at the crossing points is much less for higher ions than for lower. Thus an error in the ionization coefficients makes a much greater difference to the temperature required for a given ionization-balance ratio for highly charged ions than for lower charges. The results of the ionization-balance calculations are compared in Fig. 6 where it may be seen that at about 10^6 K, temperatures for the same population ratio are lower by about 25 per cent in the 2 × ECIP case. The differences are comparable with the differences found for example between Jordan's (1969) calculations and Summers' (1974).

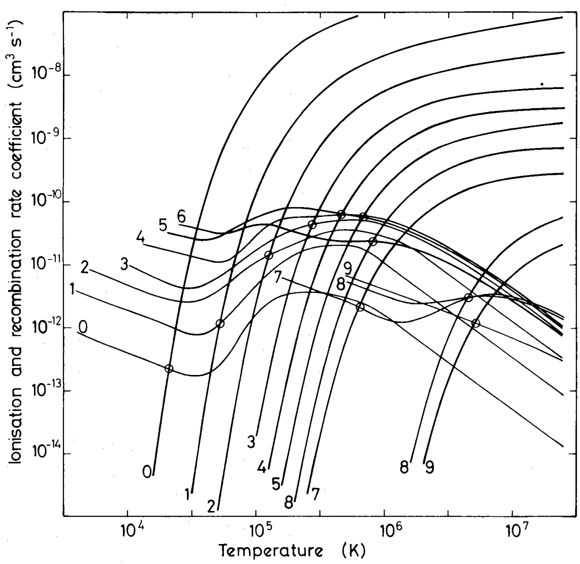

Figure 5. Ionization (ECIP × 1) and recombination rate coefficients for neon ($n_e = 10^8\,cm^{-3}$). The numbers in the curves indicate the ion charge.

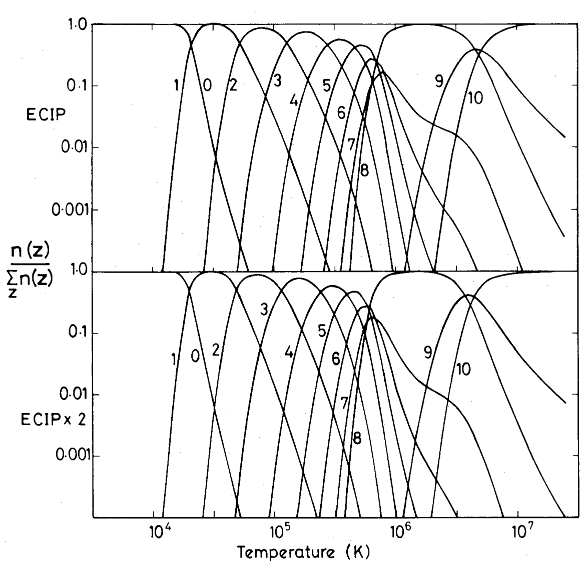

Figure 6. Comparison of the ionization balance population ratios for the ions of neon ($n_e = 10^8\,cm^{-3}$) based on ECIP ionization rates and 2 × ECIP rates.

5 Comparison of cross-sections measured by the crossed-beams method with values calculated by the Coulomb–Born approximation

A comparison of this nature has been made by Moores (1972) and covered the full available energy range. In this brief summary attention is confined to the threshold region ($E/\chi < 2$).

It is not possible to present similar comparisons for the plasma spectroscopy data since a sufficiently wide range of Coulomb–Born calculations is not available. Individual values for the ratio Coulomb–Born/Experiment are taken from Section 2 above and averaged in Table 20. The Coulomb–Born values were taken from the sources indicated in this table. Note that Moores (1972) does not include autoionization, and this strongly affects the last four ions in the table. If the effect of autoionization is applied to the Coulomb–Born results in the same way as for SEF and ECIP (see Section 1) the mean value of C–B/expt becomes 1.71 (± 23 per cent). By averaging only those to which autoionization corrections do not need to be applied the mean value of the ratio becomes 1.47 (± 24 per cent) but note the restricted nature of this sample.

Table 20.

Ion	C–B/expt	C–B Source
Na^+	2.06	Moores (1972)
Mg^+	0.97	Moores & Nussbaumer (1970)
Li^+	1.42	Moores & Nussbaumer (1970)
Mg^{2+}	1.54	Moores (1972)
He^+	1.37	Rudge & Schwartz (1966)
O^+	1.05	Moores (1972)
O^{2+}	0.87	Moores (1972)
N^{2+}	0.75	Moores (1972)
C^+	0.62	Moores (1972)

Mean values 1.18 (standard deviations ± 38 per cent)

In Fig. 3, illustrating the cross-sections for the ionization of He^+ to He^{2+}, a number of versions of the Coulomb–Born approximation are plotted. The object of this is to indicate the range of variation in results for a method that is often tacitly assumed to yield a unique solution. In the comparisons made in the tables for He^+ we have chosen the version of the Coulomb–Born approximation which corresponds with that chosen by Moores (1972).

6 Conclusion

Comparisons are made in this paper between the values for threshold ionization rates used in various ionization-balance calculations and the values measured in the laboratory. The two laboratory methods for which data are available are crossed-beams work on ionization cross-sections and plasma spectroscopy measurements of ionization rate coefficients. On average the comparisons favour the ECIP method of calculating the rate coefficients although it is not clear why this method should be superior near threshold to other simple methods. These other methods give values which are about twice those based on the ECIP method. In order, therefore, to discover the influence of such a disparity in the ionization rate coefficients on the ionization-balance calculation, the calculations of Summers (1974) were repeated for 2 x ECIP rate coefficients but with the other coefficients unaltered. This had a small effect on low stages of ionization but for ions produced at about 10^6 K, made a difference of about 25 per cent in the temperature for the same ionization balance ratio. This is comparable to the difference between calculations by Summers and by some other authors.

A comparison with Coulomb–Born calculations showed that this is no more successful than the simpler methods in calculating values that are in agreement with the measurements, although the standard deviations are smaller.

The conclusions of this paper could have important consequences for the calculation of the stage of ionization and spectrum of low-density plasmas at high temperature. It is important to note, however, that they are based on a relatively small sample of data where either (a) the ions are of small charge (crossed-beam measurements) or (b) the measurement accuracy is rather poor (plasma experiments). There is an important need to extend and improve these measurements (particularly the crossed-beam work to ions of higher charge) in order to be able to draw more reliable conclusions. There would appear also to be a need to develop better theoretical methods of calculating ionization cross-sections at threshold.

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