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Analysis of the O VIII Lyman Spectrum from a Transient
Laboratory Plasma

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ABSTRACT

The O VIII resonance spectrum occurs between 14 and 19 Å.
Measurements of the line intensities from a theta-pinch ($T_e \approx 300$ eV,
 $n_e \approx 7 \times 10^{16} \text{ cm}^{-3}$, $t \approx 1 \mu\text{sec}$) are compared with recent numerical
calculations for one-electron ions in an optically thin plasma.
Substantial agreement is obtained when the transient state of the
plasma is explicitly included.

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I. INTRODUCTION

In a recent paper¹ the line spectra of O VII and O VIII in the Scylla I, θ -pinch discharge are presented, while a previous paper² dealt with measurements of the continuum arising from electron capture by O VII, O VIII, and O IX ions. Together these data determine (a) the populations of the excited levels of the O VIII ion and their departures from the values corresponding to collisional (Saha) equilibrium with the free electrons and (b) the relative populations of the various ionization states of oxygen in the plasma and their departure from steady state values.

Recently detailed numerical calculations have been made for one electron ions in an optically thin plasma.^{3,4} They give the excited level populations for an arbitrary ground level population, as well as the steady state population of the ground level. Collisional and radiative de-excitations and collisional excitations among all levels, including the continuum, are taken into account.

The O VIII Lyman series has been remeasured and the data will be compared with the predictions of this theory. The plasma conditions which prevail for all the measurements to be reported are those corresponding to times near the maximum of the second half cycle of a deuterium discharge in the Scylla I θ -pinch. The oxygen impurity in the deuterium plasma is 12%. This represents 10% deliberately added to the filling gas, plus an estimated 2% present from the oxides of the ceramic discharge tube. The plasma temperature is 295 eV and the deuteron number density is $4.3 \times 10^{16} \text{ cm}^{-3}$.¹ The region of hot plasma occupies an ellipsoidal volume of $3 \pm 0.6 \text{ cm}^3$.³

II. MEASURED RELATIVE INTENSITIES OF THE O VIII LYMAN LINES

The most accurate measurement of the relative line intensities is that obtained with a potassium acid phthalate (KAP) diffraction crystal and a thin scintillation detector covered with a 1.5 mg/cm^2 Al foil to exclude visible light. The area under the spectral plot of each of the first five Lyman lines was measured, and the resulting intensities were corrected for the absorption of the x rays in the Al foil. These data are presented in the fifth column of table 1.

It is necessary to make a correction for the reflectivity R of the KAP crystal. This quantity was not measured for KAP, but its relative theoretical values can be given with considerable confidence over a small range of angles. These are taken from the "mosaic" formula.⁵ Assuming that the absorption coefficient μ is proportional to λ^3 ,

$$R(\lambda) \propto (1 + \cos^2 2\theta)/(2 \sin 2\theta), \quad (1)$$

where θ is the grazing angle. All lines of the O VIII Lyman series lie at angles between 31 and 45.5° . Previous absolute measurements of R on a beryl diffraction crystal⁶ showed the mosaic formula to apply quite accurately for $\theta \leq 50^\circ$. In the case of KAP there are no absorption edges to complicate the use of eq. (1). The sixth column of table 1 gives the relative intensities of the lines after correction for $R(\lambda)$.

An estimate of the errors in the relative intensities of the lines was gotten by comparing the results obtained both with the scintillation detector and with a proportional counter for the KAP crystal, and also, with those obtained for the higher members (principal quantum number $p \geq 4$) of the Lyman series with the beryl crystal. Within the errors quoted all of these measurements agree. The beryl data were normalized to the KAP measurement at $p = 6$ and are given in table 1 for $p = 7$ and 8 . Since the grazing angles are only slightly different, the relative reflectivity correction is neglected for these two entries.

III. POPULATIONS OF THE EXCITED O VIII LEVELS

The next to last column of table 1 gives the absolute intensities of the Lyman lines, scaled from measurements of the absolute continuum intensity. This is taken from fig. 3 of ref. 2 which gives $29 \text{ kW}/\text{\AA}^0$ at $14.2 \text{ \AA}$ for the case of a deuterium filling with 10% oxygen added. (The fraction of oxygen added was given as 6% in ref. 2. This assumed incorrect sensitivities of a Pirani gauge to oxygen and deuterium gases. Since then a McLeod gauge calibration has shown that the correct fraction of added oxygen was 10%. The oxygen fraction was the same in the present experiments and those of ref. 2).

Since the transition probabilities A_p of the Lyman lines are just the hydrogen values scaled up by Z^4 , the absolute intensities of the lines can be reduced to population densities of the levels according to the relation

$$n(p) = I_p / (h\nu_p A_p V), \quad (2)$$

where V is the plasma volume. The last column of table 1 gives the experimental values of $n(p)$. A statistical distribution among the sub-levels is assumed for all quantum levels $p > 2$, and the averaged A values are used. For the $p = 2$ level the transition probability between the $2p$ levels and the $1s$ ground state is greater than the collisionally induced transition rate between the metastable $2s$ level and the $2p$ levels. Therefore the A value appropriate to the $2p$ levels only is used in eq. (2) and the population thus determined applies to the $2p$ sub-levels. (We denote principal quantum number by p throughout this paper to adhere to the notation in refs. 3 and 4. To avoid confusion with the conventional designation of the angular momentum $\ell = 1$ sub-level, the use of p in this sense is always preceded by a numerical value of the principal quantum number.)

The systematic error in the absolute population densities is about 50%. This includes 40% in the absolute intensity calibration, 20% in the plasma volume and 20% in the angular window acceptance of the

spectrometer.

IV. THEORY

There are two important simplifying features in the theory of refs. 3 and 4. The first is the fact that the excited levels reach a steady state among themselves and with the completely stripped O IX ions in a time which is very short compared to that for establishing a steady state between the different ion species. This enables the excited level population to be written as the sum of a term proportional to the ground state population of the one electron O VIII ion and a term proportional to the number of stripped ions. The second feature is the existence of simple scaling laws with ionic charge Z , which enable the same calculation to be adapted to any one-electron ion. In terms of the reduced parameters, the oxygen spectrum from the hot, dense Scylla plasma is thus equivalent to a hydrogen spectrum at a density of only $4 \times 10^{10} \text{ cm}^{-3}$ and an electron temperature of five electron volts. These unusual parameters account for the differences in the solution from the conventionally encountered hydrogen spectra.

The theory gives the following expression for the population of the excited levels of O VIII in terms of the real parameters:

$$n(p) = Z^{11} f_0(p, n_e, T_e) n_{\text{IX}}/n_e + f_1(p, n_e, T_e) n(1), \quad (p \neq 1) \quad (3)$$

where f_0 and f_1 are functions of the atomic rate coefficients, which themselves are functions of electron density n_e and electron temperature T_e . In the notation of ref. 4, $f_0 = r_0(p) \eta_E(p)$ and $f_1 = r_1(p) \eta_E(p)/\eta_E(1)$. They are computed in terms of the reduced parameters.

In order to apply the theory, one needs the values of n_{IX} and $n(1)$, the number densities of O IX and the ground state of O VIII, respectively. The determination of these is the subject of the next section.

V. POPULATIONS OF THE OXYGEN IONIC SPECIES

The total number of oxygen ions of all stages of ionization is known from the total impurity concentration and the deuteron number density at peak compression. The species O I through O VI have such short lifetimes against ionization that their concentration will be completely negligible. However, on the basis of the ionization cross-sections available, the computations of refs. 7 through 9 predict a time for passage from O VII to O VIII of $\sim 3 \mu\text{sec}$ and from O VIII to O IX (no bound electrons) of $\sim 10 \mu\text{sec}$. This is much longer than the time ($0.8 \mu\text{sec}$) during which the soft x rays from these species are emitted in the present experiment. Therefore a steady state between ionization and recombination is not reached.

The relative populations of the O VII and O VIII ions can be estimated from the ratio of the instantaneous intensities of the O VII $1s^2 - 1s3p$ ($18.63 \text{ \AA}$) and O VIII L_{α} ($18.97 \text{ \AA}$) lines. In fig. 1 oscillograms of the scintillation detector signals from the O VII $1s^2 - 1s3p$ and O VIII L_{α} lines have been superimposed on a single photograph and are shown in relation to the magnetic field of Scylla I. Measurements from several oscillograms equivalent to those of fig. 1 indicate that at the time of maximum L_{α} radiation, that of O VII $1s^2 - 1s3p$, which peaks $0.3 \mu\text{sec}$ earlier, has decayed on the average by a factor of 2 and that the peak intensity of O VII is about 80% that of O VIII. Because the wavelengths are nearly identical no scaling of the photoelectric signals is necessary to compare intensities. The ratio of the O VII and O VIII line intensities at the time of peak L_{α} is, therefore, 0.4. It is self-consistent with the results to be obtained that these resonance lines arise predominantly through collisional excitation from the ground state, and therefore, their intensity is given to a good approximation by the expression

$$I = (\text{ground level population}) (\text{excitation function}) (\text{photon energy}). \quad (4)$$

Because the O VII 3p and O VIII 2p levels are at nearly equal energies

above their ground levels, the ratio of their excitation functions is to good approximation equal to that of their absorption oscillator strengths. For the O VIII L_{α} transition the hydrogen value¹⁰ $f(1s-2p) = 0.416$ is applicable. We take for the O VII transition Weiss's value:¹¹ $f(1s^2-1s3p) = 0.137$. Thus, again since the photon energies are nearly equal, one obtains for the ground level populations at the time when the O VIII L_{α} radiation peaks:

$$\begin{aligned} \frac{n_{\text{VIII}}}{n_{\text{VII}}} &\approx \frac{I(L_{\alpha})}{I(1s^2-1s3p)} \cdot \frac{f(1s^2-1s3p)}{f(1s-2p)} \\ &\approx \frac{1}{0.4} \cdot \frac{0.137}{0.416} \approx 0.8. \end{aligned} \quad (5)$$

There is no independent experimental evidence for the ratio of O VIII to O IX. Therefore, we treat

$$S = n_{\text{VIII}}/n_{\text{IX}} \quad (6)$$

as an adjustable parameter in the theory and seek the value which is consistent with the experimental data at the time the Lyman series lines peak.

Neglecting the small excited-level population densities, (see below) the sum of the ground state densities of the oxygen ionization states present is

$$n_{\text{VII}} + n_{\text{VIII}} + n_{\text{IX}} = 5.2 \times 10^{15} \text{ cm}^{-3}. \quad (7)$$

where the right hand side is the ion number density corresponding to the 12% fraction of oxygen in the compressed plasma.

Using eqs. (5), (6), and (7),

$$n_{\text{VIII}} = 5.2 \times 10^{15} S/(1 + 2.25 S) \text{ cm}^{-3}. \quad (8)$$

VI. COMPARISON WITH THEORY

A. Absolute and Relative Level Populations

Substituting eqs. (6) and (8) into (3) gives:

$$n(p) = 5.2 \times 10^{15} (Z^{11} f_o / (S n_e) + f_1) S / (1 + 2.25 S). \quad (p \neq 1) \quad (9)$$

The values of $n(p)$ were computed from the theory of ref. 4 with an IBM-7090 for the experimental conditions $Z = 8$, $T = 295$ eV, and $n_e = 4.3 \times 10^{16} (1 + 0.12 Z_{av})$. The electron density is the sum of one electron from each deuterium ion and an average number from each of the 12% oxygen ions which is a function of the parameter S . Using the observed ratio $n_{VIII}/n_{VII} = 0.8$, this is given by $Z_{av} = (8 + 14.5 S) / (1 + 2.25 S)$.

The computed function $n(p)$ is plotted in fig. 2 for various values of S . The flagged points are the experimental population densities taken from table 1. The agreement of both the absolute values and the relative variation of $n(p)$ except for $p = 2$, is very satisfactory for $S > 4$. It is to be remembered that the experimental points can be moved, besides within the flagged regions, together up or down 50% due to systematic errors in absolute value. Furthermore, the theoretical results for the low quantum numbers are relatively sensitive to the collisional excitation coefficients, which themselves are only presumed good to a factor 2.

An S value greater than 4 is quite reasonable. The same argument leading to eq. (5), applied at the instant when the O VII radiation peaks, gives a ratio of O VII to O VIII of 4.3. Since O VIII is harder to ionize than O VII, and the temperature remains essentially constant for the 0.3 μ sec between the times these radiations peak, it is to be expected that S , the ratio of O VIII to O IX at peak O VIII, will be greater than the ratio O VII to O VIII at peak O VII.

B. Discussion of Computation

In calculating $n(p)$ the total number of oxygen ions is kept fixed. If there were no O VII present, the curves would all cross at a common (non-integer) quantum number determined by a balance among the atomic rate coefficients such that the net upward transitions per O VIII ground state ion equal the net downward transitions per O IX ion. Since there is an experimentally fixed ratio 1.25 of O VII to O VIII, this cross-over actually occurs where the effect of each O VIII ion is just balanced by 2.25 O IX ions.

The actual computation assumes statistical mixing among the sub-states of the levels, including $p = 2$. The mixing rate by ion collisions of the

2s and 2p levels is still rapid compared both to changes in the ground level population and to the experimental observation time. Therefore the calculation is closely valid for the observed 2p level population if the $n(p)$ value for the entire 2 level is scaled by 0.75, the proportional amount in the 2p levels, assuming equal occupation for all sub-states.

C. Anomalous Low 2p Level Population

The complication of slow mixing of the 2s and 2p levels can not be invoked to account for the anomalously low observed value for $p = 2$. Self absorption of the Lyman α radiation as an explanation of the anomaly is also invalidated both by calculation and experiment as reported in ref. 1, where it is shown to be less than 15%.

Calculations were performed on a model in which no 2s-2p transitions are allowed and the 2s level interacts only through upward transitions to higher quantum levels. The relative fit to the lower levels was then considerably better. However, despite the fact that the 2s-2p transition rate decreases more rapidly with ionic charge Z than the electron collision rates to higher levels, the computed upward transitions for $Z = 8$ are not sufficiently rapid to justify further consideration of this model.

VII. COMPARISON WITH SAHA POPULATION DENSITIES

The populations $n_E(p)$ which the O VIII levels would have if they were in collisional equilibrium with the free electrons are given by the Saha equation:

$$n_E(p)/n_{IX} = n_e (h^2/2\pi mkT)^{3/2} p^2 \exp E(p,c)/kT. \quad (10)$$

If the plasma were in Saha equilibrium it would therefore have

$$S_E = n_E(1)/n_{IX} = 1.0 \times 10^{-7}. \quad (11)$$

The steady state solution of ref. 3 gives

$$S_s = 0.25. \quad (12)$$

This is much greater than the Saha value, because the plasma is closer to the "coronal" limit of a balance between collisional excitation from the ground state to the continuum and radiative recombination from the continuum to the ground state. Balancing only these two processes gives

$$S_c = 0.14. \quad (13)$$

The fact that the experimentally determined $S(> 4)$ is considerably greater than the steady state value implies that the O VIII - O IX system is still approaching its steady state, as discussed in Section V, when maximum plasma compression is reached.

A true Saha equilibrium plasma for the given temperature and electron density would contain oxygen practically only in the form of O IX (eq. (11)). However, given any population of n_{IX} , eq. (10) defines a "Saha equilibrium" between free electrons, completely stripped ions (n_{IX}), and the various level populations of O VIII.

In fig. 3 the ratio $R(p)$ of computed level populations to Saha equilibrium populations is plotted for various values of the parameter S for levels $p > 1$. For each value of S a new Saha population is computed, since n_{IX} is strongly, and n_e is weakly, dependent on S . The curves for $S > 4$, lying above the curve shown for $S = 4$, correspond to conditions in Scylla I up to peak compression, and that for $S = 0.25$ represents the steady state condition being approached, but never reached, in this discharge.

These curves have ratios $R(p)$ greatly in excess of unity for the lower quantum numbers because of excess collisional excitations from the ground level of O. VIII, which is vastly overpopulated compared to its Saha value. According to eq. (11), $n(1)/n_E(1) > 10^6$ for $S > 0.1$. The case for which the ground state has less than its Saha equilibrium population is illustrated by the curve $S = 0$. In this case the ratio $R(p)$ becomes less than unity because of a deficiency of collisional excitations from below.

A consequence of the "overpopulation" of the excited levels in Scylla is the qualitative appearance of the line spectra with respect to the continuum as seen in fig. 2 of ref. 2. The lines "grow" out of the continuum near the series limit, remaining well above its extrapolated

level, and the merging of their wings effectively obscures the decrease of continuum intensity at the series limit.

VIII. DEVIATIONS FROM THEORY

Despite the relatively good fit of the absolute values of the excited level populations of O VIII to the theory, some discrepancies in overall consistency with theory remain.

A. Absolute Continuum

The continuum intensity radiated per unit frequency due to recombination radiation from the capture of free electrons by O IX, directly related to the recombination coefficient utilized in the theory, can be put into the formulation given by Elwert.¹² Assuming an equivalent form for the continuum radiation from radiative capture by O VIII to form O VII (the capture by O VII to form O VI gives negligible contribution), an absolute continuum intensity is predicted, using the experimentally determined electron temperature, density, O VIII/O VII ratio, and assuming $S = 4$ for the ratio O VIII/O IX. This computed intensity is six times less than the observed intensity. If the intensity calibration uncertainty of 40% is assumed in a direction favorable to removing the discrepancy a factor four remains unexplained. (Note that a 40% decrease in absolute intensity values helps the agreement of absolute line intensities with theory in fig. 2). The major part of the continuum radiation, however, originates in the recombination to the two electron ion for which the theory is inexact, and there may also be other unrecognized contributions to the continuum.

B. Ionization Rate

The observation that the ratio O VIII/O VII changes from 0.23 to 0.8 in 0.3 μsec , implies an effective ionization rate $\langle\sigma v\rangle$ of $\sim 1.5 \times 10^{-11} \text{ cm}^3 \text{ sec}^{-1}$, compared to a value of about 3.5 times less obtained from refs. 7 and 8 by integrating the approximate ionization cross-sections for two electron ions over a Maxwellian electron velocity distribution. Again, the theoretical basis for two electron ions appears to be less well established.

IX. CONCLUSIONS

Substantial quantitative agreement between theory and experiment has been found for the resonance spectrum of O VIII in an optically thin plasma. The analysis succeeds only if the transient nature of the plasma, which has not had time to reach a steady state, is taken into account. Comparison of the experimental and computed excited level populations establishes that the ionic species depart greatly from their steady-state populations.

Table 1. Observed Intensities and Level Populations of the O VIII Lyman Series

Spectral Line	Principal Quantum Number p of Upper Level	Grazing Angle θ	Wavelength λ A	Observed Relative Intensity I_p	Relative Intensity Corrected for $R(\lambda)$	Absolute Intensity I_p (kW) ($\pm 50\%$) ^b	Population of Upper Level $n(p)$ (10^9 cm^{-3}) ^c
L_α	2	$45^\circ 30'$	18.97	1000 ± 130	1000 ± 130	600 ± 80	0.75 ± 0.10^c
L_β	3	$37^\circ 5'$	16.01	308 ± 40	274 ± 36	165 ± 22	1.95 ± 0.26
L_γ	4	$34^\circ 48'$	15.18	80 ± 11	67 ± 9	40 ± 5.5	1.96 ± 0.27
L_δ	5	$33^\circ 52'$	14.82	25 ± 4	20 ± 3	12 ± 1.8	1.77 ± 0.27
L_ϵ	6	$33^\circ 24'$	14.64	8.2 ± 1.3	6.5 ± 1	3.9 ± 0.6	1.42 ± 0.22
L_ζ^a	7	$65^\circ 30'$	14.53	3.2 ± 0.5	3.2 ± 0.5	1.9 ± 0.3	1.50 ± 0.24
L_η^a	8	$65^\circ 6'$	14.46	1.6 ± 0.3	1.6 ± 0.3	1.0 ± 0.2	1.54 ± 0.29

a. Beryl data

b. The uncertainty range listed applies to the relative values between the lines. The further 50% range on absolute value is discussed in the text.

c. The observed intensity gives directly only the population of the 2p states, as discussed in the text.

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CAPTIONS

- Fig. 1. Scintillator signals of diffracted x rays from the O VII $1s^2 - 1s3p$ and O VIII L_{α} lines. The two x-ray signals were taken on successive discharges and superimposed on a single oscillogram by shifting the base line.
- Fig. 2. Comparison of the experimentally determined electron population densities of the O VIII levels with those computed from the theory of refs. 3 and 4. The computed curves are parameterized in S, the ratio of the O VIII to O IX ion density.
- Fig. 3. Ratio $R(p)$ of excited level populations to Saha equilibrium populations for various values of S, the ratio of O VIII to O IX ion density.

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Fig. 1

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