Validity criteria for local thermodynamic equilibrium in plasma spectroscopy

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We have solved the collisional-radiative equations for atomic hydrogen and hydrogenlike ions (of nuclear charges 2 and 26) in a plasma and derived their excited-state populations for a wide range of plasma temperatures and densities. The populations of the higher-lying levels are well described by the Saha-Boltzmann equation. We refer to such plasmas as being in partial local thermodynamic equilibrium (LTE), and it is the purpose of this paper to present expressions by which it is possible to predict the lowest principal quantum number that meets the criterion of being within 10% of its Saha-Boltzmann value. We treat the ionizing plasmas, the recombining plasmas, and the plasmas in ionization balance as three separate cases. These criteria are then extended to the ground state to cover plasmas in complete LTE. Finally we discuss briefly the effect of opacity on these results and the extent to which they may be used for non-hydrogen-like systems. Throughout the paper care is taken to present physical pictures to explain the numerical results and comparisons are made with LTE criteria derived using more qualitative arguments by other authors.

I. INTRODUCTION

The concept of local thermodynamic equilibrium (LTE) has been widely used to simplify the interpretation of spectral line intensities from laboratory and some astrophysical plasmas. Thus it has been possible to develop spectroscopic methods for the determination of electron temperature T_e and density n_e. It is also important in experimental atomic physics, e.g., in the determination of atomic transition probability from an observation of the line intensity. Thus, there are many circumstances where it is important to have rather precise criteria to identify the plasma conditions under which it is safe to assume LTE in order to carry out a successful analysis.

The standard definition of LTE is that the population density of quantum level p should be described by the Saha-Boltzmann equation, viz.,

$$n_{\rm SB}(p)=[n(g)]^+ n_e \frac{g(p)}{2[g(g)]^+}\left(\frac{h^2}{2\pi m k T_e}\right)^{3/2}\exp\left(\frac{\chi(p)}{kT_e}\right) \tag{1}$$

$$=[n(g)]^+ n_e Z(p) , \tag{1a}$$

where $n_{\rm SB}(p)$ and $g(p)$ are the Saha-Boltzmann population density and the statistical weight, respectively, of level p, $[n(g)]^+$ and $[g(g)]^+$ are the population density and the statistical weight, respectively, of the ground state g of the ion having charge greater than that of level p by 1, $\chi(p)$ is the ionization potential of level p, k is Boltzmann's constant, and the other symbols have their usual meanings. We will refer to $Z(p)$ as the Saha-Boltzmann coefficient and define complete LTE as the situation where the populations of all the levels of the atom or ion are described by Eq. (1).

It is also useful to use the concept of partial LTE where only a limited range of levels can be described by the Saha-Boltzmann equation (1). It is well known from the theory of collisional-radiative processes that the upper levels of an ion reach a thermal distribution with the continuum of free electrons more easily than the lower levels. Thus, we will define the levels of the ion as being in partial LTE from level p if Eq. (1) applies to it and all higher-lying levels.

For the purpose of illustration, we take hydrogen atoms or hydrogenlike ions as a model of atomic systems. We assume the statistical population density distribution among the different l and j sublevels (except where otherwise stated), and p is used to denote the principal quantum number of this level. Griem[1] proposed a criterion for partial LTE. His argument was based on the comparison between the radiative decay rate and the collisional depopulation rate from the same level. Let $A(p,q)$ be the radiative transition probability from p to q, $C(p,q)$ the collisional excitation $(q>p)$ rate coefficient, $F(p,q)$ the deexcitation $(q<p)$ rate coefficient, and $S(p)$ the ionization rate coefficient. For level p to be in partial LTE, the collisional depopulation rate should be greater than, say by ten times, the radiative decay rate, i.e.,

$$\left[\sum_{q\,(>p)} C(p,q)+\sum_{q\,(<p)} F(p,q)+S(p)\right]n_e \ge 10 \sum_{q\,(<p)} A(p,q) . \tag{2}$$

For p much larger than 1 or for high temperatures, the dominant collision processes are excitation, and Eq. (2) is approximated to

$$n_e \ge 10 \sum_{q\,(<p)} A(p,q) \Big/ \sum_{q\,(>p)} C(p,q) n_e . \tag{3}$$

Relation (3) is numerically given as

$$p \geq 82(T_e/z^2)^{1/17}(n_e/z^7)^{-2/17} \ , \tag{4}$$

where n_e is measured in cm^{-3}, T_e is in K, and z is the nuclear charge of the ion under consideration.

Other workers have proposed criteria for partial LTE; Wilson[2] defined the thermal limit, which was equivalent to the critical level for partial LTE, and gave a numerical expression for the quantum number of this level. McWirter[3] started with a somewhat different reasoning and derived a slightly different criterion. Drawin[4] refined the approximation to the excitation cross section or the excitation rate coefficient in Eq. (3), and modified Eq. (4).

In discussing the rate of recombination of an afterglow plasma, Byron *et al.*[5] defined the "bottleneck" level as the one that has the minimum of $n_{\text{SB}}(p)F(p,p-1)$. The quantum number of this level is expressed by

$$s=(z^2R/3kT_e)^{1/2} \ , \tag{5}$$

where R is the ionization potential of the ground-state hydrogen atom or the Rydberg constant, and the levels lying higher than this level were assumed to be in LTE. Thus, for level p to be in partial LTE,

$$p \geq s \tag{6}$$

should be met. Hinnov and Hirshberg[6] also proposed a similar criterion to Eq. (5); the factor 3 is absent in their criterion.

In 1973 Fujimoto[7] and Engelhardt[8] independently pointed out that there can be conditions under which the criteria expressed by Eqs. (4) and (6) are fulfilled and still excited-state populations deviate from the Saha-Boltzmann values [Eq. (1)]. Their arguments are based on the formulation of the collisional-radiative model[9] as follows: Let $b(p)$ be the reduced population density defined by

$$b(p)=n(p)/n_{\text{SB}}(p) \ . \tag{7}$$

In this model, the excited-state population is expressed as

$$b(p)=r_0(p)+r_1(p)b(1) \tag{8}$$

for $p \geq 2$, where $r_0(p)$ and $r_1(p)$ are called the population coefficients which are determined from the collisional and radiative atomic processes taking place in the plasma, and are functions of n_e and T_e. There can be conditions such that the second term is dominant, and the excited-state populations are determined by this term which is proportional to the ground-state population. Thus, depending on the magnitude of $b(1)$, the resulting population can be much higher than Eq. (1), or $b(p) \gg 1$, even if the criteria such as in Eq. (4) are met. The assertions of Fujimoto and Engelhardt are supported by several experiments: e.g., even if Eqs. (4) and (6) are satisfied, the excited-state populations in a positive-column argon plasma are almost independent of n_e, obviously violating the LTE properties,[10] and the excited-state populations in a transient plasma deviate appreciably from their LTE values for a hydrogen plasma[11] and for a helium plasma.[12]

Griem[1] also gave a criterion for complete LTE. When all the collisional transitions between the ionic levels predominate over the competing radiative transitions, the thermal population distribution is extended to all levels including the ground state. Then, the critical density is given by

$$F(2,1)n_e \geq 10A(2,1) \ , \tag{9}$$

or numerically,

$$n_{\text{es}}=9.8\times10^{14}z^7(T_e/z^2)^{1/2} \ \ (\text{in cm}^{-3}) \ . \tag{10}$$

In view of the practical importance of the concept of LTE, it is necessary to establish a set of validity criteria for establishing partial and complete LTE. In this paper we first summarize the physical ideas behind these existing criteria and extend them into new areas before making detailed comparisons with the results of full collisional-radiative calculations for optically thin plasmas of hydrogen ($z=1$), helium ions of charge 1 ($z=2$), and iron ions of charge 25 ($z=26$). In this way we will be able to identify the limits of the ranges of LTE with good reliability for hydrogen and hydrogenlike ions. We start by discussing partial LTE and find it convenient to divide plasmas into recombining, ionizing, and ionization-balance plasmas. We also discuss complete LTE. The application of the results to non-hydrogen-like species is discussed briefly as is the question of applicability in optically thick conditions.

II. GENERAL CONSIDERATIONS

It is convenient to divide the plasmas that we are going to be concerned with into three different classes depending on whether they are recombining, ionizing, or are in ionization balance.[13] We define a recombining plasma as one where the population density of the ground state is less than its value in ionization balance, $n_{\text{IB}}(1)$, as calculated by the collisional-radiative theory for the local values of T_e, n_e, and n^+ (which we use instead of $[n(g)]^+$) [see Eq. (22)]:

$$b(1)<b_{\text{IB}}(1)=n_{\text{IB}}(1)/n_{\text{SB}}(1) \ . \tag{11}$$

When condition (11) is met the plasma is in a dynamic state with the electrons recombining with fully stripped ions to eventually form ground-state atoms or ions.

In a similar way we define an ionizing plasma as one where the ground-state population is greater than what it would be in the ionization balance:

$$b(1)>b_{\text{IB}}(1) \ . \tag{12}$$

When the plasma is in a steady state and uniform, the ionization ratio of the plasma is determined solely by the ionization-recombination rates of the plasma and is in ionization balance; i.e., $b(1)=b_{\text{IB}}(1)$. In many cases, however, the plasma is not in a steady state and uniform, and therefore, the ionization-balance plasma is a rather exceptional case.

Since we confine ourselves at this stage to hydrogen atoms and hydrogenlike ions, it is convenient to express the results in terms of the reduced electron temperature Θ and electron density η as suggested by Bates *et al.*[9] [see Eqs. (4), (5), and (10)],

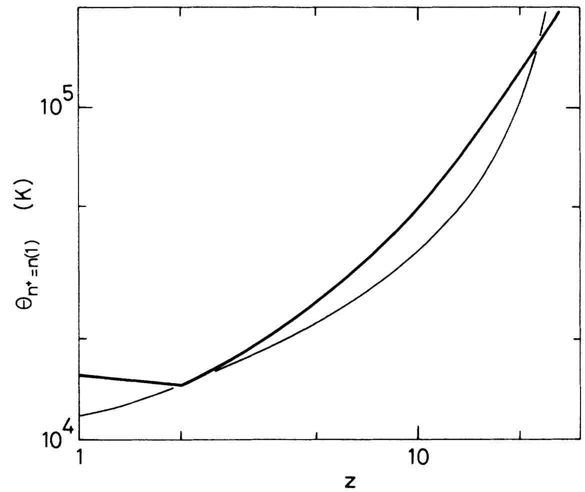

FIG. 1. The temperature at which $n^+=n_{\rm IB}(1)$ for a plasma in ionization balance. Electron density is $\eta=10^{10}$ cm^{-3}. Thick curve: result of numerical calculation. Thin curve: approximate expression derived in Ref. 25. See Appendix A.

$$\Theta=T_e/z^2 \ \text{(in K)}, \quad \eta=n_e/z^7 \ (\text{in cm}^{-3}) . \tag{13}$$

In this way the major differences between the ions are removed and the results show more clearly the remaining differences.

For a plasma in ionization balance having a constant electron density, the condition under which the emission-line intensities show maximum values is determined by its temperature. This temperature approximately coincides with the temperature at which the populations of the ground-state and the fully stripped ions are equal,[14] or $n_{\rm IB}(1)=n^+$. Figure 1 shows the appropriate range of temperature Θ at which $n_{\rm IB}(1)=n^+$ holds for ions of nuclear charge $1\le z\le 26$ for a reduced electron density $\eta=10^{10}$ cm^{-3}. (See Appendix A.) These values of Θ are relatively insensitive to the electron density. For example, at $\eta=10^6$ cm^{-3} and $z=10$, Θ is within 2% of the values at 10^{10} cm^{-3}, and at $\eta=10^{14}$ cm^{-3} it is within 25%. This suggests that it is necessary to cover quite a wide range of temperatures Θ for the present study to be useful. We have chosen the range $1\times10^3\le\Theta$ $(=T_e)\le1.28\times10^5$ K for atomic hydrogen and $4\times10^3\le\Theta(=T_e/z^2)\le5.12\times10^5$ K for hydrogenlike ions.

We illustrate the way in which the populations of the excited states vary. In the formulation of the collisional-radiative model the excited-state population is expressed as a sum of the two terms given by Eq (8). For a recombining plasma the value of $b(p)$ lies between $r_0(p)$ and the ionization-balance value $b_{\rm IB}(p)$. In Fig. 2 we show examples of these values calculated by the collisional-radiative treatment as described later, as a function of p for various temperatures and densities for atomic hydrogen and hydrogenlike ions. Except for cases of very high temperature the values of $r_0(p)$ are equal to or less than unity so that recombining plasmas tend to have values of $b(p)$ that are closer to unity than this limiting value. Note, however, that for values of Θ greater than about 2.5×10^5 K some values of $r_0(p)$ are greater than unity as illustrated in Fig. 2(c). This may be of importance for the recombination of very highly charged ions ($z\gtrsim30$). We note in passing that the low-density limiting position of the $r_0(p)$ curves is the so-called capture-cascade solution and depends only on radiative processes.

For an ionization-balance plasma it may be seen that $b_{\rm IB}(p)$ is very close to or greater than unity and that at large values of p it always approaches unity asymptotically.

For an ionizing plasma $b_{\rm IB}(p)$ represents the lower limit of $b(p)$ so that the population densities of the excited levels of these plasmas depart from their Saha-Boltzmann values, $b(p)=1$, to a greater or lesser extent depending on the instantaneous population density of the ground state, $b(1)$. Thus, it is clear from these curves that the criteria for partial LTE must, in addition to the electron temperature and density, depend on the value of the ground-state population.

It may also be seen that sometimes the population densities of quite low levels may "accidentally" meet the requirement of Eq. (1) because of the complex shape of the curves, but this does not meet the spirit of our definition of partial LTE. This point is illustrated in Fig. 2(a) by the thick dotted curve for $\Theta=4\times10^3$ K, $\eta=10^{10}$ cm^{-3}, and $b(1)=9\times10^6$ instead of $b_{\rm IB}(1)=1.7\times10^7$. It shows that although level $p=3$ meets the definition (1) this plasma nevertheless does not meet the full requirement that all levels above it should also satisfy Eq. (1). It is not until level $p=11$ that the criterion [see Eq. (15)] is satisfied.

Figure 2 includes the ground-state population $b_{\rm IB}(1)$ for the plasma in ionization balance. For sufficiently high density, it is seen that all the discrete states (including the ground state) enter into LTE, or $b_{\rm IB}(p)=1$ for $p\ge1$. This situation is called complete LTE, as defined in Sec. I.

III. PARTIAL LTE

A. Criterion for n_e

According to our definition of partial LTE, the excited-state population with which we are concerned should be closely connected with the continuum-state populations. More specifically, the populating process to this level should start from the continuum states, and the depopulating process terminate on these states, even if these connections may be indirect as is almost always the case. For this situation to be realized, the first requirement is that the collisional depopulating transition(s) from this level should predominate over the radiative decay from this level. This requirement is identical to that proposed by Griem[1] and other workers[2-4] [Eq. (2)], and therefore, the specific formula for this condition should be Eq. (4) or its equivalent.

B. Criterion for T_e

In this high-density plasma that satisfies the first requirement, it may be shown that the dominant collisional transitions from or to other levels are excitation or deexcitation, both from or to the adjacent levels and that other transitions, such as the direct ionization from this level and the three-body recombination to this level, are always unimportant compared with these transitions. (See Figs. 3–7 of Ref. 15, Figs. 3–7 of Ref. 16, and Figs. 4–7 of Ref. 17.) Thus, there are four possible combinations of the dominant populating and depopulating processes of this level as schematically illustrated in Fig. 3. It is obvious that among these four cases only the case of Fig. 3(b) leads to partial LTE, because only in this case is there a possibility that this population is thermally related to the continuum-state populations.

For this to be realized the dominant depopulating pro-

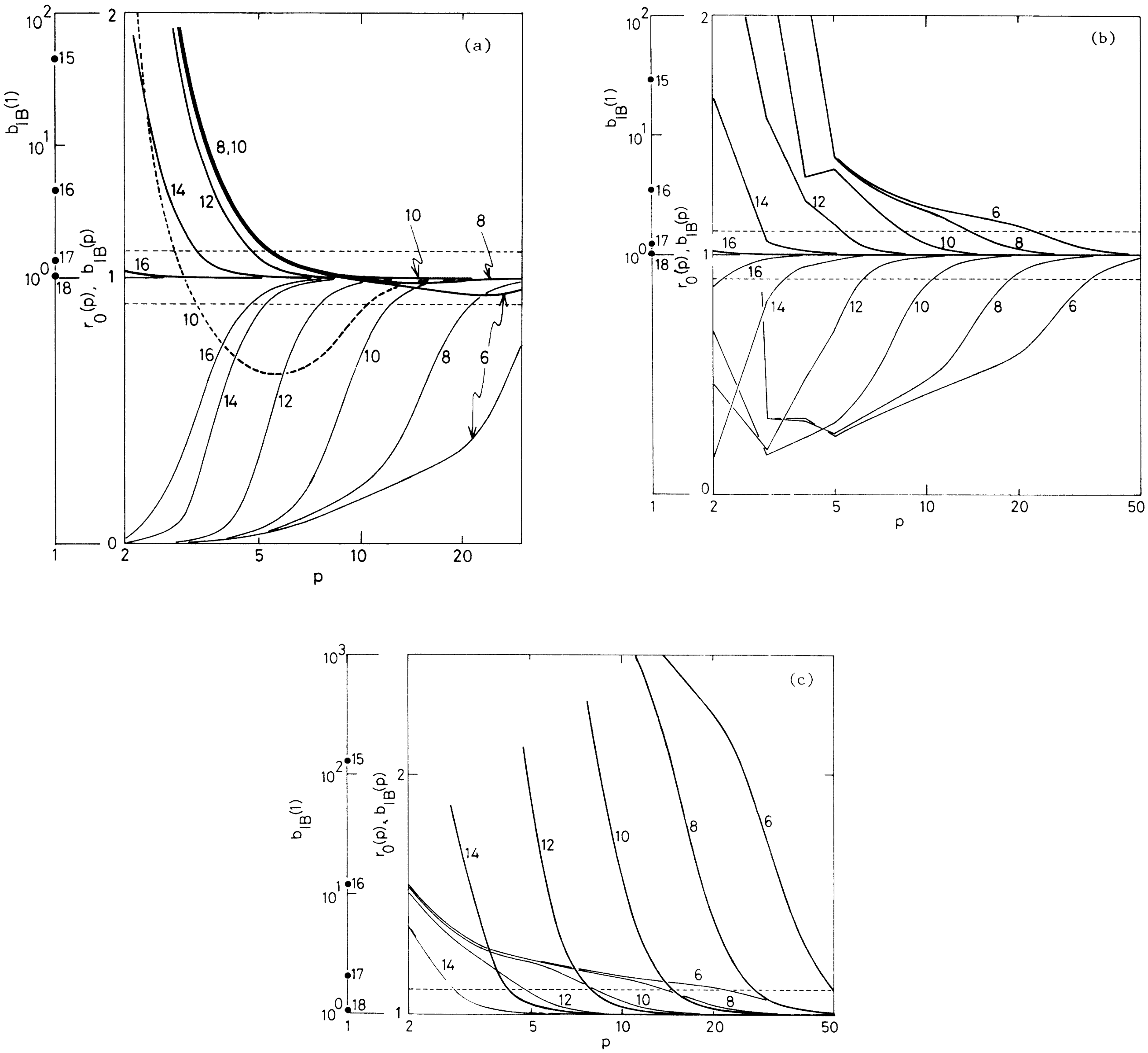

FIG. 2. The population coefficient $r_0(p)$ (thin solid curves), which represents the population in complete recombining plasma, and the reduced population $b_{IB}(p)=r_0(p)+r_1(p)b_{IB}(1)$ for plasma in ionization balance (thick solid curves). The numbers in the figure indicate the power of 10 of the reduced electron density η measured in cm^{-3}. The two horizontal thin dashed lines indicate the boundary of the LTE populations, i.e., 1 ± 0.1 [Eqs. (15) and (16)]. The closed circles on the left ordinate represent the reduced population density of the ground-state atoms or ions in ionization balance. (a) Atomic hydrogen ($z=1$), $\Theta=T_e=4\times10^3$ K. The thick dotted curve shows the population densities in slightly recombining plasma for $n_e=10^{10}$ cm^{-3} with $b(1)=9\times10^6$ instead of $b_{IB}(1)=1.65\times10^7$. See text for more detail. (b) Hydrogenlike helium ($z=2$), $\Theta=1.6\times10^4$ K. In this calculation the different l and j sublevels are resolved for levels of $2\leq p\leq 4$, and the averaged value of the coefficients and the populations over these sublevels are given. Owing to the existence of the metastable $2s$ level, some values of $r_0(2)$ for low densities are greater than 1. (c) Hydrogenlike iron ($z=26$), $\Theta=5.12\times10^5$ K.

cess should be the excitation $p \rightarrow p+1$, rather than the deexcitation $p \rightarrow p-1$, or[7,17]

$$C(p,p+1) \geq F(p,p-1) \ . \tag{14}$$

This leads to an approximate analytical expression[7,17] that is identical to Eq. (6) with Eq. (5), or

$$\Theta \geq R/3kp^2 \ . \tag{14a}$$

C. Criterion for $b(1)$

The above two requirements specify the population scheme required for the case of Fig. 3(a) or 3(b). In order to exclude the case of Fig. 3(a), we need a requirement that specifies the ground-state population. This requirement is concerned with the overall ionization balance of the system, or deviations from it, and is not expressed in terms of n_e or T_e. Instead, we have to consider to which class of plasma this particular system belongs.

The above three requirements may be interpreted in terms of the collisional-radiative model represented by Eq. (8); for $b(p)$ to be close to unity the third requirement states that the second term $r_1(p)b(1)$ should be sufficiently small compared with the first term $r_0(p)$. Then, it is obvious that the first requirement is that the electron density should be high enough so that $r_0(p)$ reaches its limiting value.[18] The second requirement states that this limiting value should be close to unity.[18]

It is noted that the above requirements are adequate only for partial LTE. For establishment of complete LTE, it is not necessary to meet requirements (14) or (14a). (See Sec. V.)

In the next section we discuss these requirements in a quantitative way, and derive specific expressions.

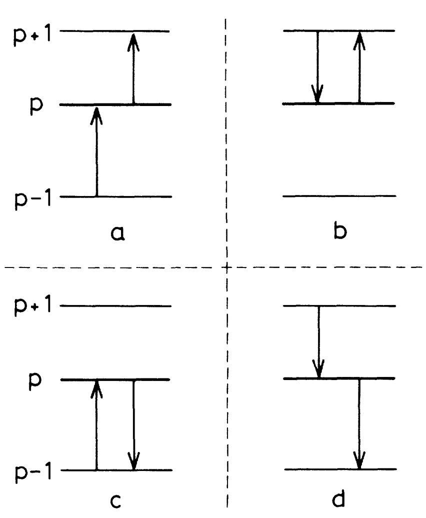

FIG. 3. Schematic diagram of the four possible cases of the dominant populating and depopulating processes of level p in which we are interested, under high-density conditions where the radiative transitions are neglected.

IV. SPECIFIC CRITERIA FOR PARTIAL LTE

In this section we perform a full collisional-radiative model calculation for atomic hydrogen and hydrogenlike ions, and use the result to derive a set of validity criteria for partial LTE along the line outlined in the preceding section. We define LTE as the situation in which the population lies in the range of 10% above or below the Saha-Boltzmann value, Eq. (1), or the reduced population $b(p)$ must lie in the range

$$0.9 \leq b(p) \leq 1.1 \ . \tag{15}$$

A. Collisional-radiative model

For neutral hydrogen and hydrogenlike ions, rate constants for radiative recombination and spontaneous radiative decay are exact, and we installed these in our computer programs.

For ionization and excitation cross sections of neutral hydrogen by electron collisions we relied primarily on the experimental data whenever possible. We also relied on the relationship between the cross section for excitation from the ground state to Rydberg states, and that for ionization.[19] We slightly modify the structure of the semiempirical formulas proposed by Johnson[20] to fit the cross sections which we believe to be the best choice at present. The details are given in the Appendix B. The effect of proton collisions is neglected. The excited states having the principal quantum number smaller than 36 are included in the calculation.

The collisional-radiative model developed for the hydrogenlike ions is called COLRAD, and its details are described in Refs. 21–23. This can be applied to ions with the nuclear charge z in the range $2 \leq z \leq 35$. The atomic parameters which do not exactly obey the z scaling, from which Eq. (13) has been derived, are the excitation- and ionization-rate coefficients. The results of the calculations show some dependence on z. The number of excited states included in the calculation may be chosen freely, and sometimes excited states as high as $p=100$ are included (usually $p=50$).

For $p=2$, 3, and 4 the l and j sublevels were calculated specifically within the program, i.e., they were not assumed to be populated statistically. In calculating the rates of collisions between them account was taken of proton collisions. In fact, for the conditions with which this paper is concerned, departures from statistical populations for these levels made no significant difference.

B. Recombining plasma

First we consider a class of plasmas where the second term of Eq. (8) is entirely neglected; this may be called the completely recombining plasma.[13,16,17] As has been noted in Sec. II, $r_0(p)$ asymptotically tends to unity with increasing p. The validity criterion may be expressed as

$$0.9 \leq r_0(p) \leq 1.1 \ . \tag{16}$$

In Fig. 2 we identify the quantum number p_R of the critical level which meets the requirement (16). In Fig. 4 we plot p_R for a wide range of temperature with density as a parameter. We give noninteger values of p_R because of the continuous properties of $r_0(p)$ as a function of p, and the values close to $p_R=2$ may contain some ambiguities. The salient features are (i) with the exception at temperatures about $\Theta=2.5\times10^5$ K, p_R depends only slightly on Θ but strongly on η. (ii) At temperatures around 2.5×10^5 K, all of the excited states satisfy Eq. (16) even if density is very low. This is a result of a coincidence between the magnitudes of the populating flow to level p, i.e., $\sum_{q(>p)} n(q)A(q,p)+\beta(p)n^+n_e$, and the depopulating flow, i.e., $\sum_{q(<p)} A(p,q)$ as discussed in detail in Ref. 16 (p. 1563). Here $\beta(p)$ is the radiative recombination rate coefficient to the level p. (iii) For low temperatures low-lying levels never enter partial LTE even if the density becomes high. This may be understood from the discussion in Sec. III B that in high-density plasma the requirement (14) or (14a) should be met for temperature. For lower temperatures, the electrons do not have enough collision energies to return the electron bound in level p to level $p+1$; rather, the dominant process is the deexcitation $p \to p-1$ as schematically illustrated by Fig. 3(d) (see also Fig. 7 of Ref. 17). In Fig. 4 we also give the lower end of the levels for which Eqs. (3) and (4) hold, for $\eta=10^8$ cm^{-3}, as an example for atomic hydrogen. The original LTE criterion describes the overall feature of $r_0(p)$ rather well except at low temperatures.

We now try to establish an empirical formula which expresses the above results more exactly. From numerical fitting we find that the values of p that satisfy condition (16) may be represented by

$$p \geq 118/\Theta^{0.43}+279/\eta^{0.15} \tag{17}$$

and

$$p \geq 282/\Theta^{0.5} . \tag{17'}$$

In Fig. 4 the critical level given by Eq. (17) and (17′) is shown with the thin solid curves and the thin dotted line, respectively. It is interesting to note that the density dependence of Eq. (17), $\propto \eta^{-0.15}$, is similar to the criteria such as Eq. (4), $\propto \eta^{-0.118}$ and discussed in Sec. I. The relationship of Eq. (17′) has a similarity to Byron's expression, Eqs. (5) and (6); the right-hand side of Eq. (17′) may be expressed as $(R/2k\Theta)^{1/2}$ where the factor 2 is different from his value of 3.

As can be seen from the comparison of Eq. (17) and the result of the numerical calculation in Fig. 4, this equation gives a rather conservative estimate. If our plasma has a high temperature such that the second term of Eq. (17) is the decisive term, the lower end of the LTE levels would be lower, and Eq. (17) should be accordingly relaxed by a certain amount.

Figure 5 is another plot of the same data as Fig. 4 and is constructed from the three cases of $z=1$, 2, and 26. It identifies the region of Θ and η for various p_R. The region to the right of each curve corresponds to the range of Θ and η in which the levels lying higher than p_R are in partial LTE.

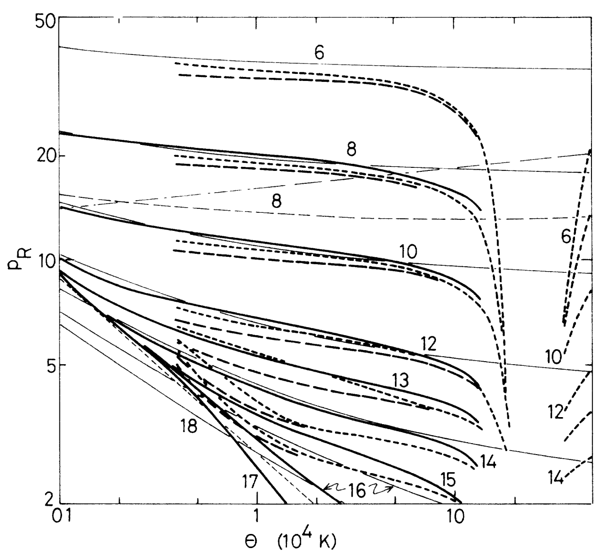

FIG. 4. The principal quantum number of the critical level p_R for establishment of partial LTE in recombining plasma for a wide range of temperature. The thick curves are the result of numerical calculation. ——: $z=1$. ----: $Z=2$. — — —: $z=26$. ——: Eq. (17). ----: Eq. (17a). — — —: critical level for which Eq. (3) holds for atomic hydrogen. —·—·—: Eq. (4). The numbers in the figure indicate the power of 10 of reduced electron density η in units of cm^{-3}.

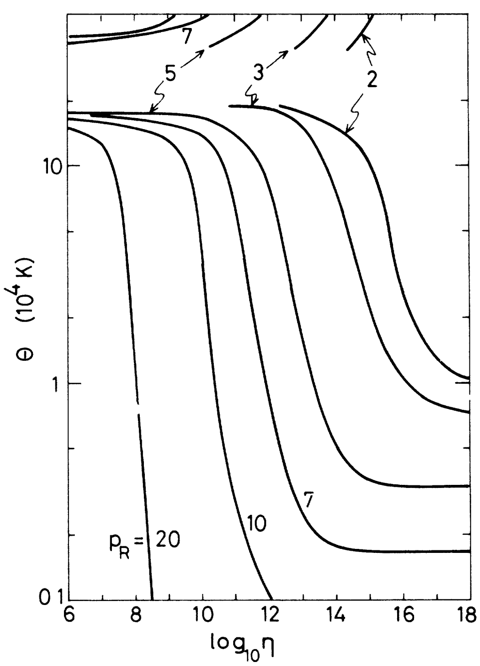

FIG. 5. The principal quantum number of the critical level p_R in the η-Θ plane for recombining plasma. The region to the right of a curve is the region of density and temperature in which the higher-lying levels than the critical level are in LTE. This figure is constructed from the three cases ($z=1$, 2, and 26) in Fig. 4, and therefore only approximate.

C. Plasma in ionization balance

We start with the plasmas of low density; this is for the purpose of understanding the population characteristics in these plasmas in relation to the Saha-Boltzmann distribution.

We first consider the plasmas with high temperatures. The first term of Eq. (8), $r_0(p)$, is, at low densities, close to unity. [See in Fig. 2(c) the case of $10 \lesssim p \lesssim 20$ for $\eta = 10^6$ cm^{-3}. See also the numerical tables in Refs. 9, 18, or 24 and the discussion in Refs. 7 and 16.] This is the reason why the lower end of partial LTE, p_R, for the recombining plasma goes down for $\Theta \simeq 2.5 \times 10^5$ K. It was also shown[13] (see also Appendix A) that the ratio of the two terms $[r_1(p) b_{IB}(1)/r_0(p)]$ is of the order of 10. Thus, in the high-temperature cases, the population is larger than, but not far from, the Saha-Boltzmann value. Figure 2(c) shows an example.

We next consider a very-low-temperature atomic hydrogen plasma. In Appendix B we show that the threshold value of the excitation cross section is closely related to the slope of the ionization cross section just above the ionization threshold. We also note that the radiative decay probability from very-high-lying levels is also related to the radiative recombination of low-energy continuum electrons. It then follows that the population density of very-high-lying levels, represented by $r_1(p) b_{IB}(1)$ in Eq. (8), is close to $\frac{2}{3}$. The first term, $r_0(p)$, is about $\frac{1}{3}$. (See the numerical tables of Refs. 9, 18, or 24.) Therefore, the resulting population $b_{IB}(p)$ is close to unity. Figure 2(a) contains examples (see the case of $10 \lesssim p \lesssim 20$ for $n_e = 10^6$ cm^{-3}).

Thus, for practically any temperature, the populations of high-lying excited states in the low-density limit are not far from the Saha-Boltzmann values, and when the electron density is finite, these populations are brought close to the equilibrium values, $b_{IB}(p) = 1$, starting from higher-lying levels. Figure 6, which corresponds to Fig. 4, shows the critical level p_{IB} for partial LTE as determined from Fig. 2. It is seen that for temperatures lower than 3×10^4 K the critical level p_{IB} is lower than that for recombining plasma p_R. This is understood as follows: For low temperatures, $r_0(p)$ is smaller than unity. The second term $r_1(p) b_{IB}(1)$ tends to help $b_{IB}(p)$ come close to unity. On the other hand, for higher temperatures the critical level is higher than that in the recombining plasma. This is because, in these cases $r_0(p)$ is rather close to unity for any temperatures and densities, and for $\Theta > 2.5 \times 10^5$ K they are even larger than unity. [See Figs. 2(b) and 2(c).] The addition of the second term makes it more difficult for $b_{IB}(p)$ to be close to unity than $r_0(p)$ itself.[25] Figure 7, which corresponds to Fig. 5, shows the region of density and temperature for establishing LTE. From numerical fitting we find a formula for p that satisfies the LTE condition

$$p \geq 85 \Theta^{0.1} / \eta^{0.133} . \tag{18}$$

The lower end p_{IB} determined by Eq. (18) is shown in Fig. 6 by the thin solid lines. In Fig. 6 the lower end for the LTE criterion, Eq. (3) or (4), is shown for $\eta = 10^8$ cm^{-3} as an example. It is seen that these formulas are reasonably good.

D. Ionizing plasma

As has been mentioned in Sec. II, the second term of the right-hand side of Eq. (8) could be the dominant term, and $b(p)$ could be much larger than unity as suggested from Fig. 2. When the electron density is high, this situa-

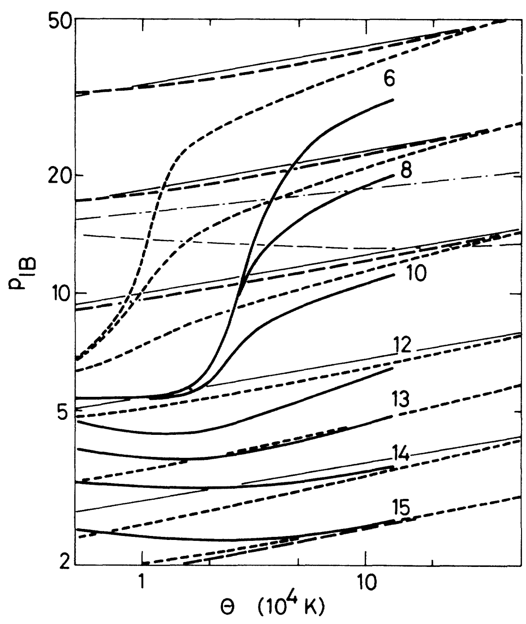

FIG. 6. The critical level for partial LTE in ionization-balance plasma, corresponding to Fig. 4. The explanation is the same as for Fig. 4.

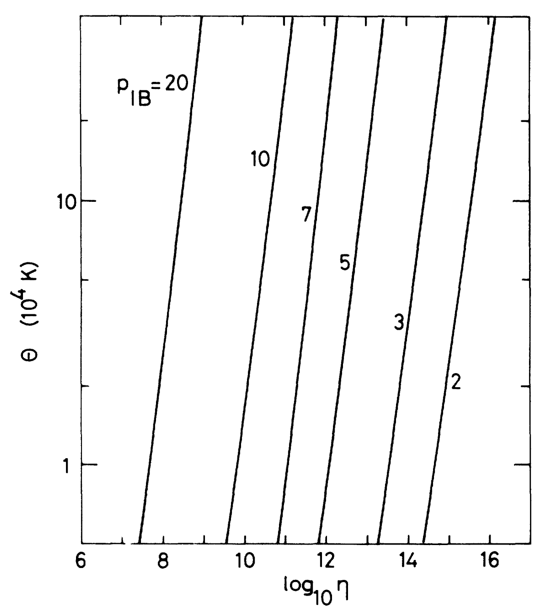

FIG. 7. The same as Fig. 5, but for ionization-balance plasma.

tion corresponds to the population scheme as depicted by Figs. 3(a) or 3(c). However, if the ground-state population, or $b(1)$, is not large enough, $b(p)$ for large p still could lie within the LTE criterion [Eq. (15)].

We start with the assumption that our plasma has high temperature, i.e., $\Theta \geq 3\times10^4$ K, and high density, i.e., $\eta \geq 1\times10^{15}$ cm^{-3}. Under these conditions we have approximations of $r_0(p)=1$ within 30% and

$$r_1(p)=p^{-6} \tag{19}$$

within a factor of 2. (See the numerical tables of Refs. 9, 18, or 24 and the discussion in Refs. 7, 16, and 18.) Figure 8 shows examples of $r_1(p)$ for several cases including those violating the above assumption of high temperature and density. This simple minus-sixth-power distribution of the excited-state population is a result of the establishment of the multistep ladderlike excitation-ionization scheme among the discrete levels.[15] (See Fig. 7 of Ref. 15.) Roughly speaking, $n(p)C(p,p+1)n_e$ is independent of p, and the p dependence of $C(p,p+1)\propto p^4$ makes the population $n(p)\propto p^{-4}$, or $n(p)/g(p)\propto p^{-6}$. In order for level p to be in LTE, it is obvious from Eq. (8) and from the discussion in Sec. III C that the contribution from the second term should be sufficiently small, or specifically

$$r_1(p)b(1)\leq 0.1 \tag{20}$$

should hold. In approximation (19), requirement (20) is expressed as

$$p \geq [10b(1)]^{0.167} . \tag{21}$$

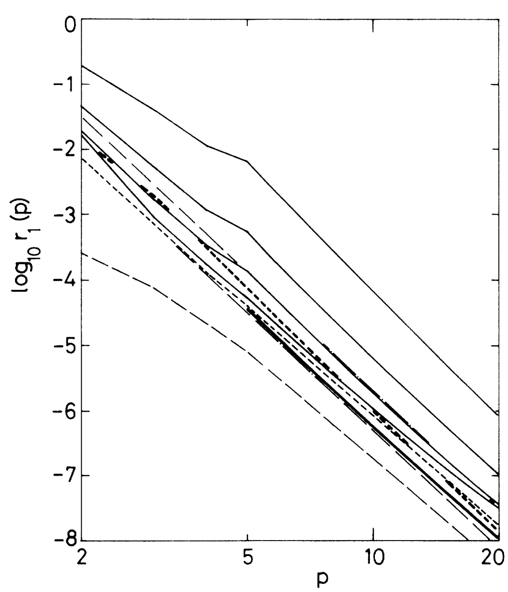

FIG. 8. The population coefficient $r_1(p)$ against p. ----: $z=1$, $\eta=10^{17}$ cm^{-3}, and $\Theta=3.2\times10^4$ K. ——: $z=1$, $\eta=10^{17}$ cm^{-3}, and $\Theta=1.28\times10^5$ K. ——: $z=2$, $\eta=10^{17}$ cm^{-3}, from top to bottom $\Theta=8\times10^3$, 1.6×10^4, 3.2×10^4, and 5.12×10^5 K. ----: $z=2$, $\eta=10^{15}$ cm^{-3}, and $\Theta=5.12\times10^5$ K. — — —: $z=2$, $\eta=10^{13}$ cm^{-3}, and $\Theta=5.12\times10^5$ K. —·—·—·: $p^{-6}\times2$ and $p^{-6}/2$.

Table I compares Eq. (21) with the results of numerical calculations for several plasma conditions which include those violating our requirements. For plasmas meeting our requirements, levels lower lying than Eq. (21) have a population density distribution of $n(p)/g(p)\propto p^{-6}$.

For densities lower than 1×10^{15} cm^{-3}, $r_1(p)$ becomes smaller than p^{-6} [see Fig. 8 of this paper and Fig. 1 of Ref. 15; remember that, for low densities, the excited states are in the corona phase and $r_1(p)$ is proportional to η], and criterion (21) gives too stringent an estimate. Table I(e) gives an example. For lower temperatures $r_1(p)$ becomes larger than p^{-6} as seen in Fig. 8, and Eq. (21) is too relaxed. Table I(f) gives an example. Howev-

TABLE I. The critical level p_l for establishment of partial LTE in ionizing plasma. Numbers in brackets denote powers of 10.

(a) $\Theta=3.2\times10^4$ K, $\eta=10^{15}$ cm^{-3}				
	$z=1$	$z=2$	$z=26$	
$b(1)$	$b_{IB}(1)=8.53[1]$	$b_{IB}(1)=3.78[1]$	$b_{IB}(1)=2.58[1]$	Eq. (21)
10^2	2.6	2.9	3.2	3.2
10^4	6.4	7.2	7.3	6.8
10^6	13.2	15.1	16.2	14.8
(b) $\Theta=3.2\times10^4$ K, $\eta=10^{17}$ cm^{-3}				
	$z=1$	$z=2$	$z=26$	
$b(1)$	$b_{IB}(1)=1.71[0]$	$b_{IB}(1)=1.33[0]$	$b_{IB}(1)=1.22[0]$	Eq. (21)
10	2.2	2.2	2.3	2.2
10^3	4.9	5.3	5.3	4.7
10^5	10.1	11.1	11.6	10.0
(c) $\Theta=5.12\times10^5$ K, $\eta=10^{15}$ cm^{-3}				
	$z=1$	$z=2$	$z=26$	
$b(1)$	$b_{IB}(1)=1.49[2]$	$b_{IB}(1)=1.35[2]$	$b_{IB}(1)=1.31[2]$	Eq. (21)
10^3	4.2	4.3	4.3	4.7
10^5	9.4	9.7	9.8	10.0
10^7	21.5	22.5	22.6	21.7
(d) $\Theta=5.12\times10^5$ K, $\eta=10^{17}$ cm^{-3}				
	$z=1$	$z=2$	$z=26$	
$b(1)$	$b_{IB}(1)=2.24[0]$	$b_{IB}(1)=2.12[0]$	$b_{IB}(1)=2.09[0]$	Eq. (21)
10	2.0	2.0	2.0	2.2
10^3	4.4	4.5	4.5	4.7
10^5	9.8	10.1	10.1	10.0
(e) $\Theta=2.56\times10^5$ K, $\eta=10^{13}$ cm^{-3}				
	$z=1$	$z=2$	$z=26$	
$b(1)$	$b_{IB}(1)=2.12[4]$	$b_{IB}(1)=1.88[4]$	$b_{IB}(1)=1.82[4]$	Eq. (21)
10^5	7.0	7.2	7.3	10.0
10^7	15.6	16.5	17.0	21.7
10^9	36[a]	39.0	41.0	46.8
(f) $\Theta=1.6\times10^4$ K, $\eta=10^{17}$ cm^{-3}				
	$z=1$	$z=2$	$z=26$	
$b(1)$	$b_{IB}(1)=1.60[0]$	$b_{IB}(1)=1.25[0]$	$b_{IB}(1)=1.15[0]$	Eq. (21)
10	2.7	2.6	2.7	2.2
10^3	6.0	6.5	6.5	4.7
10^5	12.2	13.7	14.5	10.0

[a]Extrapolated.

er, such a low-temperature case is unlikely to be realized in actual ionizing plasmas.

V. COMPLETE LTE

The concept of complete LTE implies that the plasma is in a temporal steady state and that it is uniform. Later in this section we will examine the extent to which these requirements may be relaxed and still meet the criterion that we adopt, i.e., that all values of $b(p)$ lie in the range of $0.9 \leq b(p) \leq 1.1$ including now $p=1$.

In the theory of the collisional-radiative model, the effective rates for ionization and recombination of the system are described by the collisional-radiative ionization-rate coefficient S_{CR}, and the recombination rate coefficient α_{CR}, both being functions of n_e and T_e. The ionization balance relation is then given as

$$n^{+}/n_{\mathrm{IB}}(1)=S_{\mathrm{CR}}/\alpha_{\mathrm{CR}} \; . \tag{22}$$

In the high-density limit these rate coefficients are in the internal relationship

$$\alpha_{\mathrm{CR}}=S_{\mathrm{CR}}Z(1)n_e \; . \tag{23}$$

It has also been shown that in this high-density region the population coefficients $r_0(p)$ and $r_1(p)$ are in their high-density limits and they are in another internal relationship (Refs. 7, 13, and 18; see also tables of Refs. 9, 18, or 24),

$$r_0(p)+r_1(p)=1 \; . \tag{24}$$

This relation together with Eqs. (22) and (23), or $b_{\mathrm{IB}}(1)=1$, substituted into Eq. (8) leads to $b_{\mathrm{IB}}(p)=1$ for all $p(\geq 2)$. Thus, complete LTE is established.

In Fig. 9, the critical density η_s, at which $b_{\mathrm{IB}}(1)=1.1$ holds, is given as a function of temperature for $z=1$, 2, and 26. The criterion [Eq. (10)] gives a reasonably good estimate for ions, but a gross underestimate for atomic hydrogen. We define the criterion as

$$\eta \geq \eta_s \; , \tag{25}$$

with

$$\eta_s=1.5\times 10^{18}(\Theta/10^6)^a \tag{26}$$

and

$$a=0.55-(0.49/z)^{1.5} \; . \tag{27}$$

The critical density is shown by the thin solid lines. The densities corresponding to $10A(2,1)/F(2,1)$ and $10\beta(1)/\alpha(1)$ are also given for atomic hydrogen for the purpose of comparison. For lower temperatures the critical density is determined by the former quantity through the density dependence of S_{CR}, because α_{CR} reaches its limiting value at much lower density.[17] For higher temperatures η_s is determined by the latter through α_{CR}, because the critical density for S_{CR} is determined by the former quantity which is smaller.

As noted above, for a plasma to be in ionization balance it should be uniform and steady state. In practice, however, these ideal requirements cannot be met, and we must establish practical limits. We first consider a time-dependent plasma. In order for this plasma to be in complete LTE, the "time lag" of $n(1)$ from $n_{\mathrm{SB}}(1)$, which is determined by the instantaneous values of n_e, n^+, and T_e, should be small. In view of the practical importance, we first assume a pure hydrogen plasma, that is, $n^+=n_e$ and $n(1)+n^+=N$. The above requirement [Eq. (25)] is assumed for electron density. The rate equation for ionization-recombination is

$$\frac{d}{dt}n(1)=-S_{\mathrm{CR}}n(1)n_e+\alpha_{\mathrm{CR}}n^{+}n_e \; . \tag{28}$$

It is straightforward to show that the relaxation time τ for this system is given by

$$\tau^{-1}=(S_{\mathrm{CR}}+\alpha_{\mathrm{CR}})n_e \; . \tag{29}$$

We envisage a situation in which the number density N and T_e vary with time and deviation of the densities from their stationary values is small. It is straightforward to show that the temporal variation of $n_{\mathrm{IB}}(1)$, or that of $n^+=n_e$, is given as a sum of two terms which stem, respectively, from the temporal variation of N and that of T_e:

$$\frac{dn_e}{dt}=\frac{1}{2Z(1)n_e+1}\left[\frac{dN}{dt}+\left[\frac{3}{2}+\frac{z^2R}{kT_e}\right]\frac{Z(1)n_e^2}{T_e}\frac{dT_e}{dt}\right] . \tag{30}$$

Now we require that the temporal variation of the stationary quantities should be sufficiently slow as compared with the relaxation time of this system:

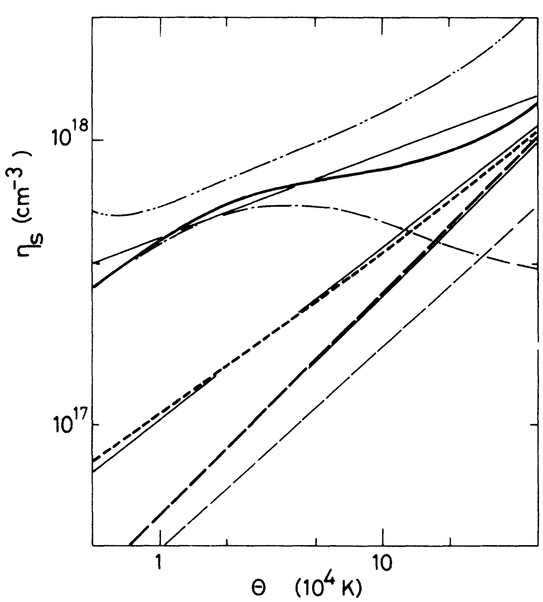

FIG. 9. Critical electron density for establishment of complete LTE. Thick curves show the results of numerical calculation. ——: $z=1$. ----: $z=2$. — — —: $z=26$. ——: Eq. (25) with Eq. (26). — — —: Eq. (10). —·—·—: $10A(2,1)/F(2,1)$. —··—··—: $10\beta(1)/\alpha(1)$.

$$|\dot{n}_e|/n_e \leq 0.1\tau^{-1} , \tag{31}$$

where the dot denotes the time derivative. We assume Eq. (25) is already met and use Eq. (23), where we adopt the approximate expression for S_{CR} in this high-density limit,[25]

$$S_{CR} \simeq 1\times10^{-7}\exp(-3z^2R/4kT_e)/z^3 , \tag{32}$$

which is valid for $\Theta > 1\times10^4$ K. We require that Eq. (31) be met by the time variations of N and T_e independently. Then we have

$$|\dot{N}|/N \leq 1\times10^{-8}[2Z(1)n_e+1]\exp(-3R/4kT_e)n_e \tag{33}$$

and

$$|\dot{T}_e|/T_e \leq 1\times10^{-8}\frac{[2Z(1)n_e+1][Z(1)n_e+1]}{(\frac{3}{2}+R/kT_e)Z(1)} \times\exp(-3R/4kT_e) . \tag{34}$$

When our system is a minority component such as an impurity in a plasma a change in plasma parameters should be slow enough for our ions to be in complete LTE. We define the reduced Saha-Boltzmann coefficient

$$Z'(p)=Z(p)z^3 = \frac{g(p)}{2[g(g)]^+}\left[\frac{h^2}{2\pi mk\Theta}\right]^{3/2}\exp\left[\frac{R}{p^2k\Theta}\right] ; \tag{35}$$

then the following conditions should be met:

$$|\dot{n}_e|/n_e \leq 1\times10^{-8}[z^4Z'(1)\eta+1]^2 \times Z'(1)^{-1}\exp(-3R/4k\Theta) \tag{36}$$

and

$$|\dot{T}_e|/T_e \leq 1\times10^{-8}\frac{[z^4Z'(1)\eta+1]^2}{(\frac{3}{2}+R/k\Theta)Z'(1)}\exp(-3R/4k\Theta) . \tag{37}$$

We now consider a plasma which is steady state but not uniform. Here again we assume the situation in which deviation of the plasma from complete LTE is small. In the preceding equations we may simply replace the time derivative d/dt by the spatial derivative $v(d/dr)$, where v is the average speed of the diffusion motion of the particles of the system under consideration.

VI. DISCUSSION

In the majority of the foregoing calculations we have assumed the statistical population distribution among different l and j sublevels of a given p. The validity criterion for this assumption has been discussed by several workers, and numerical expressions are given in Ref. 26 for various conditions. An example of the formula is

$$p \geq 59z^{0.059}/\eta^{0.118} , \tag{38}$$

which assumes light ion (proton) collisions and is valid for $p<5$ and ions with $Z\leq25$. When Eqs. (17) and (18) are compared with Eq. (38) it is seen that, under plasma conditions at which Eq. (17) or (18) is crucial, Eq. (38) is well satisfied in almost all cases. An example is seen in Fig. 2(b).

So far we have assumed that the plasma is optically thin, or more specifically, reabsorption of emission radiation does not affect the population dynamics of the atoms or ions. In this section we consider the cases in which this assumption breaks down and discuss necessary modifications to the results derived in the previous sections.

For optically thick plasmas, the equation of radiation transport should be solved simultaneously with the rate equations for the population densities. However, sometimes it is adequate to adopt an approximation that a reduced transition probability for the spontaneous transition describes the effect of reabsorption of the line. In the following we proceed in this approximation.

Optical thickness of an absorption line is proportional to the lower-level population, the absorption oscillator strength, and the dimension of the plasma, and inversely proportional to the line width. A common situation would be that the resonance line, the Lyman-α line, is optically thick or has a high optical thickness, and other members of the Lyman-series lines and the Lyman continuum are optically thick to some extent. In some cases the lines terminating on excited states, especially the first excited state, are also optically thick.

For a recombining plasma the effect of reabsorption of Lyman lines is rather simple. An extreme case, the case B, is sometimes considered in which the Lyman-series lines are completely optically thick, and the transition probability $A(p,1)$ is assumed to be 0 for all p. In this case, two effects result: (i) The critical density corresponding to Eq. (3), or the second term of the right-hand side of Eq. (17), decreases owing to the effective decrease in the radiative decay probability of the excited level; (ii) the value of $r_0(p)$ increases in the lower-density regions as a result of the decrease in the radiative decay rate and an increase in the populating rate from other excited levels. For large p the decrease in the critical density is about 25%, and in Eq. (17) we may replace the factor 279 by 270, i.e., the effect is minimal. When the lines terminating on excited states also become optically thick the above two effects become larger, and the criterion on density is further relaxed.

In the optically thick plasma, the value of $r_1(p)$ also increases by the similar effects to those for $r_0(p)$. The ionization rate coefficient S_{CR} also increases as a result of the enhanced $r_1(p)$ for excited levels.[18] Therefore, for an ionization-balance plasma the effect of radiation reabsorption is complicated; necessary modifications to the criterion depend on to which lines and how strongly the radiation reabsorption takes place.

The effect of reabsorption of radiation in high-temperature plasma helps the critical density decrease above which the approximation $r_1(p)=p^{-6}$ is valid, and the criterion [Eq. (21)] becomes valid for lower densities.

As is easily seen, the validity criterion for complete LTE [Eq. (25) with Eq. (26)] is relaxed. However, its extent depends on to which lines and how strongly the radiation reabsorption takes place.

We now consider cases of atoms and ions that are not hydrogenlike. It is a well known fact that, for high-lying states in a series and having different principal quantum numbers, the energy-level structure is well approximated with the hydrogenic energy levels with an effective (noninteger) principal quantum number p^*. Various characteristics of the atomic states are sometimes approximated fairly well by those of the hydrogenic states, and the population characteristics are also expected to be approximated by those of the hydrogenic atoms and ions, with which we have been concerned. However, it is more difficult to realize the statistical population distribution among the different l, j, and core states in these cases, and the critical density for the statistical distribution is higher than that given by Eq. (38). This critical density, however, is usually lower than the density given by Eq. (3), because this statistical equilibration is established mainly through dipole transitions between the states lying rather close in energy. Therefore, for densities higher than the critical density given by Eq. (3) the population coefficient $r_0(p^*)$ is expected to be well approximated by the hydrogenic $r_0(p)$, which is exemplified in Fig. 2. For a recombining plasma the criterion [Eqs. (17) and (17′)] is expected to be approximately valid for non-hydrogen-like cases.

For lower densities than the above critical density, the population coefficient $r_1(p^*)$ and the collisional-radiative ionization coefficient S_{CR}, as well as their relationships in magnitudes, are different from the hydrogenic case. For instance, in the case of neutral helium in a low-density plasma the contribution from the metastable- to excited-state populations is sometimes much larger than that from the direct excitation from the ground state. Therefore, for the ionization-balance plasma the LTE criterion would strongly depend on the species with which we were concerned.

Several experiments appear to support that, for higher densities than the critical density, the p dependence of $r_1(p^*)\propto(p^*)^{-6}$ is well obeyed for atomic species other than hydrogenic ones.[10,12,27,28] Furthermore, Fig. 3(a) of Ref. 12 indicates that, for neutral helium of an ionizing plasma with $T_e=4.5\times10^4$ K and $n_e=1\times10^{14}$ cm^{-3}, the experimentally determined population coefficient is $r_1(n\,^3D)=0.047(p^*)^{-6}$, which compares with $0.17(p^*)^{-6}$, where the factor $0.17=[R/\chi(1\,^1S)]^{-3}$ accounts for the nonhydrogenic ionization potential of the ground state. This deviation by the factor 3.6 may be attributed to the fact that the density of this plasma is rather low (1×10^{14} cm^{-3}) for the establishment of Eq. (19) (see Fig. 8). Therefore, in many atomic and ionic systems in a high-density plasma the population coefficient $r_1(p^*)$ appears to be well approximated as $r_1(p^*)=[R/\chi(g)]^{-3}(p^*)^{-6}$, where g denotes the ground state. If this were the case, the criterion [Eq. (21)] with a necessary modification is applicable to these atomic and ionic systems. It is strongly hoped that experimental and theoretical investigations are done that examine whether the above approximation is valid for many atomic and ionic systems.

VII. CONCLUSION

In this paper we have presented practical expressions by which it is possible to predict if the populations of the excited states of hydrogen atoms or hydrogenlike ions contained in a plasma can be adequately described by the Saha-Boltzmann equation. We distinguish the situation where only a limited number of upper levels fall within this regime and the other where it applies to all states including the ground state. The first we call partial local thermodynamic equilibrium and the second complete LTE. Since LTE is a theoretical concept that can never be exactly met in practice we have chosen the practical condition for our atoms or ions to fall within the definition of LTE: i.e., their populations must be within 10% of the corresponding Saha-Boltzmann values. The criteria have been calculated by solving the collisional-radiative equations for atomic hydrogen on the one hand, and hydrogenlike ions of nuclear charge 2 and 26 on the other, and comparing the results with the corresponding Saha-Boltzmann values. On this basis we have derived formulas that represent the validity criteria. For partial LTE it has been convenient to divide plasmas into three classes where (i) it is in a state of active recombination, (ii) it is in ionization equilibrium (i.e., steady-state ionization balance), and (iii) it is actively ionizing. In each class we have determined the value of the lowest principal quantum number p of the excited levels meeting our LTE criterion. For a recombining plasma there are two criteria that must both be met, viz.,

$$p\geq118/\Theta^{0.43}+279/\eta^{0.15} \tag{17}$$

and

$$p\geq282/\Theta^{0.5}\ , \tag{17'}$$

where the equation numbers give reference to the appropriate part of the text of the paper.

For a plasma in ionization balance our criterion is

$$p\geq85\Theta^{0.1}/\eta^{0.133}\ . \tag{18}$$

For a plasma that is in a state of active ionization to be in partial LTE it must be of high temperature ($\Theta\geq3\times10^4$ K) and high density ($\eta\geq10^{15}$ cm^{-3}) and in addition satisfy the criterion

$$p\geq[10b(1)]^{0.167}\ . \tag{21}$$

For complete LTE our criterion is

$$\eta\geq1.5\times10^{18}(\Theta/10^6)^a\ , \tag{25}$$

where

$$a=0.55-(0.49/z)^{1.5}\ . \tag{27}$$

In deriving these criteria we have taken care to describe the physical reasons for them. Thus it is possible to understand how they might be extended to atoms and ions that are not hydrogenlike. We also give a qualitative discussion of the effect of radiation trapping and point to the need for experimental confirmation of our theoretical predictions.

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APPENDIX A: PLASMA IONIZATION BALANCE AND ITS SCALING LAW

In this appendix we discuss several important properties of the plasma in ionization balance and its scaling law against the nuclear charge z.

In the theory of the collisional-radiative model the effective rate of ionization and that of recombination are described by the collisional-radiative ionization-rate coefficient $S_{\rm CR}$ and recombination rate coefficient $\alpha_{\rm CR}$. According to the scaling of the reduced electron temperature $\Theta = T_e/z^2$ and density $\eta = n_e/z^7$, the reduced rate coefficients are $S_{\rm CR}/z^3$ and $\alpha_{\rm CR} z$. It then follows that the reduced "ionization ratio" is $[z^4 n^+/n_{\rm IB}(1)]$. This means that for constant Θ and η and a varying z, the "ionization ratio" is not constant but is

$$n^+/n_{\rm IB}(1) \propto z^{-4} . \tag{A1}$$

The first point is that, for a constant reduced temperature and a varying z, even though the above "ionization ratio" has the strong z dependence, the relative contributions from the two terms in the right-hand side of Eq. (8) are approximately independent of z. This will be shown below.

In the limit of low density the population corresponding to the second term is described by corona equilibrium

$$n_1(p) \simeq C(1,p) n_{\rm IB}(1) n_e \Big/ \sum_{q\,(<p)} A(p,q) , \tag{A2}$$

and the first term is given by the capture-cascade scheme

$$n_0(p) \simeq \beta(p) n^+ n_e \Big/ \sum_{q\,(<p)} A(p,q) . \tag{A3}$$

In these expressions the cascade contributions have been neglected, which are as much as 30% for high temperatures and more for low temperatures. The "ionization ratio" is given by

$$n^+/n_{\rm IB}(1) = S(1) \Big/ \sum_{q\,(\geq 1)} \beta(q) . \tag{A4}$$

The ratio of the two terms is

$$n_0(p)/n_1(p) \simeq \beta(p) S(1) \Big/ C(1,p) \sum_{q\,(\geq 1)} \beta(q) . \tag{A5}$$

In the approximation that the bound-free Gaunt factor is unity, $\beta(q)$ can be expressed as

$$\beta(q) = \frac{2^6}{3\sqrt{3}} \frac{\sqrt{\pi} e^4}{m^2 c^3} \frac{1}{q^3} \left[\frac{R}{kT_e} \right]^{3/2} \times \exp\left[\frac{R}{q^2 kT_e} \right] \left[-\mathrm{Ei}\left[-\frac{R}{q^2 kT_e} \right] \right] , \tag{A6}$$

where the exponential integral may be approximated to

$$-\mathrm{Ei}(-x) \rightarrow \begin{cases} -\ln x - \gamma , & x \ll 1 \quad \text{(A7)} \\ e^{-x}/x , & x \gg 1 \quad \text{(A8)} \end{cases}$$

where $\gamma = 0.5772$ is Euler's constant.

We first consider the case of high temperature. For a large q, $\ln q$ may be approximated to $0.7\sqrt{q}$, and roughly speaking, $\beta(q) \propto q^{-2.5}$ for $q \geq 1$. The excitation and ionization rate coefficients are proportional to the oscillator strengths for the respective transitions, and for excitation from the ground level we have $C(1,p) \propto p^{-3}$. The oscillator strength for the $1 \rightarrow 2$ transition is approximately equal to that for the $1 \rightarrow$continuum transition, and therefore we have $C(1,2) \simeq S(1)$. It then follows that the ratio (A5) is of the order of 0.1, being independent of z.

The above fact also justifies the common practice of assuming corona equilibrium for the excited-state population by neglecting the contribution from the recombining plasma component $n_0(p)$. It is further noted that, under this condition, the first term in the right-hand side of Eq. (8), $r_0(p)$ (which is usually neglected in practice), is close to 1, as discussed in Sec. IV B.

When the temperature is very low, the rate coefficients for excitation and ionization from the ground state are determined by the cross-section values close to their thresholds. A relationship between these cross-section values is discussed in Appendix B for the case of neutral hydrogen. The approximate relationship between the rate coefficients is thus given by

$$\frac{C(1,p)}{2p^{-3}} \Big/ S(1) = \frac{R}{kT_e} \exp\left[\frac{R}{p^2 kT_e} \right] . \tag{A9}$$

The population given by Eq. (A2) is expressed as

$$n_1(p) \simeq n^+ n_e \frac{\sum_{q\,(\geq 1)} \beta(q)}{\sum_{q\,(<p)} A(p,q)} \frac{2R}{p^3 kT_e} \exp\left[\frac{R}{p^2 kT_e} \right] . \tag{A10}$$

For lower-lying levels than $q \simeq 10 \sim 20$, we adopt the second approximation, Eq. (A8) for $\beta(q)$, and we have

$$\sum_{q\,(\geq 1)} \beta(q) \simeq \frac{2^6}{3\sqrt{3}} \frac{e^4}{m^2 c^3} \left[\frac{\pi R}{kT_e} \right]^{1/2} \delta , \tag{A11}$$

where

$$\delta = \sum_{q=1}^{10\sim 20} q^{-1} \tag{A12}$$

is of the order of 3. For the higher-lying levels with which we are concerned the radiative decay probability is approximated, on the assumption that the bound-bound

Gaunt factor is unity, by

$$\sum_{q\,(<p)} A(p,q) \simeq \frac{2^7}{\sqrt{3}} \frac{\pi e^2}{h^2 m c^3} R^2 \frac{\ln p}{p^5} . \qquad \text{(A13)}$$

Here,

$$\ln p = \int_1^p q^{-1} dq \qquad \text{(A14)}$$

is of the order of 3. It is concluded that, in the present approximation, Eq. (A2) is close to two-thirds of the Saha-Boltzmann value [Eq. (1)], or $r_1(p) b_{\rm IB}(1) \simeq \frac{2}{3}$. It may be also shown that, under these conditions, $r_0(p)$ is not far from $\frac{1}{3}$. An example of the exact calculation is shown in Fig. 2(a). (See the case of $10 \lesssim p \lesssim 20$ for $n_e = 10^6$ cm^{-3}.) The ratio of the two terms does not strongly depend on z.[29]

We next consider a consequence of the scaling law [Eq. (13)]. As discussed in Sec. II, for a varying temperature the "ionization ratio" $[n^+/n_{\rm IB}(1)]$ is important in determining the emission-line intensity, or the excited-state population $n(p)$ with $p \geq 2$. Since $n(p)$ takes the maximum approximately at a temperature at which $[n^+/n_{\rm IB}(1)] = 1$ hold,[14] we call the latter temperature the optimum temperature. It is clear from the discussion at the beginning of this appendix that the reduced optimum temperature has a z dependence. In Ref. 25 an approximate expression for this temperature has been derived for low-density plasma,

$$\Theta = (R/k)(13.5 - 4 \ln z) . \qquad \text{(A15)}$$

Figure 1 contains this approximation.

APPENDIX B: EXCITATION AND IONIZATION CROSS SECTIONS FOR ATOMIC HYDROGEN

The excitation cross section from the ground state to the first excited state is well established experimentally and theoretically. The cross section to higher-lying levels is not well known. In a recent experiment on a tokamak plasma to determine the atomic and molecular hydrogen densities in it,[30] it has been concluded that the cross sections given by the semiempirical formula by Johnson[20] lead to a more reasonable result than those from the recent 15-state R-matrix calculation[31] do.

In Ref. 19 the process of collisional excitation and that of ionization are discussed on the common basis of the extended Wannier classical theory, and the relationship between the excitation and ionization cross sections is established theoretically as well as experimentally.

In the present study we proceed as follows: We fit the ionization cross section derived in the above theory to the experimental data[32] which are well established (Fig. 10). By the use of the above relationship, the cross section for excitation to Rydberg states is determined, as shown in Fig. 10. The cross-section values just above the threshold are not determined in this theory, but it is suggested that they are about a factor of 2 larger than the values at higher energies.[19] The part of the cross section shown with the thick dotted curve is smaller than the result of the numerical calculation by as much as 20%.

We slightly modify the structure of the semiempirical cross-section formula by Johnson for excitation and that for ionization. The excitation cross section is expressed as

$$\sigma_{q,p}(U_{q,p}) = \frac{2q^2}{x} U_{p,q}^{-1} [1 + s_{q,p} \exp(-r_{q,p} U_{q,p})] \times \left[A_{q,p} \left[\ln U_{q,p} + \frac{1}{2U_{q,p}} \right] + \left[B_{q,p} - A_{q,p} \ln \frac{2q^2}{x} \right] \left[1 - \frac{1}{U_{q,p}} \right] \right] \pi a_0^2 , \qquad \text{(B1)}$$

where $U_{q,p}$ is the incoming electron energy in threshold units and x is the energy difference of these levels in Rydberg units. $A_{q,p}$ and $B_{q,p}$ are the parameters in the Born approximation, and a_0 is the first Bohr radius. The parameter $s_{q,p}$ is absent in the original Johnson's formula and determines the cross-section value near the excitation threshold. We also add a similar adjustable parameter s_q to the ionization cross-section formula. In the original formula, these quantities were effectively set equal to -1. We adjust these quantities very slightly so as to obtain a reasonable fit to the cross sections which have been mentioned above; for ionization $s_1 = -0.59$, and for excitation $s_{1,p} = -0.95$ for $2 \leq p \leq 5$ and $s_{1,p} = -0.9$ for $p \geq 10$. In Fig. 10 the cross sections given by these modified formulas are shown with the thin solid curves. In this figure

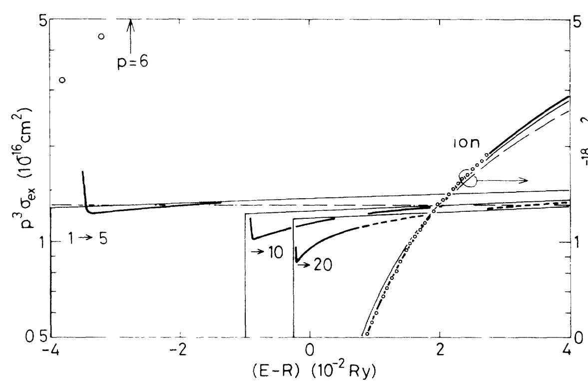

FIG. 10. Excitation and ionization cross sections from the ground state of neutral hydrogen by electron collisions in the energy range close to the ionization threshold. The excitation cross section has been multiplied by p^3. ∘∘∘: experimental ionization cross section (Ref. 32). ——, ----: cross sections derived in Ref. 19 and fitted to the experimental ionization cross section. —·—·—·: cross sections in the relationship of Eq. (B2) and fitted to the experimental ionization cross section. ——: the modified semiempirical formula (B1) for excitation and the similar formula for ionization and fitted to the most reliable experimental and theoretical data. ○: the 15-state R-matrix calculation of the excitation cross section 1→5 (Ref. 31). The arrow with "$p=6$" indicates the excitation threshold of level $p=6$.

a few values of the cross section $\sigma_{1,5}$ given by the R-matrix calculation[31] are shown for energies lower than the threshold of the $p=6$ states, where the neglect of the existence of the higher-lying states in this calculation do not affect the result.

We now discuss an approximate relationship between the ionization and excitation cross sections introduced above. We concentrate our attention on the energy range very close to the ionization threshold. We approximate the excitation cross section to be constant ($\sigma_{1,p}=\sigma_0 \propto p^{-3}$) and the ionization cross section to be a linear function [$\sigma_{\text{ion}}=\alpha(E-R)$]. We now assume smooth continuation from the excitation of Rydberg states across the ionization limit to ionization. More specifically, the rate at which electrons are raised to the discrete states having energies of $-\Delta E<E<0$ (ΔE is small) is assumed equal (except for the Boltzmann factor) to that at which continuum electrons having energies of $0<E<\Delta E$ are produced. Then it is straightforward to derive the relationship

$$\alpha=\sigma_0/(2R/p^3) \; . \tag{B2}$$

In Fig. 10 the ionization cross section as given by $\alpha(E-R)$ is shown with the thin dash-dotted curve, which tends to the modified Johnson's formula near the ionization threshold. The value of $\sigma_0 p^3$ ($=1.3\times10^{-16}$ cm^2) thus determined from this ionization cross section and Eq. (B2) is shown with the dash-dotted line. It is seen that the above approximation is good to within 20–30 %.

For excitation and ionization cross sections from excited states there are several calculations and a few experiments, and we employ the semiempirical formula by Johnson[20] in its original form for the low-lying levels and that by Vriens and Smeets[33] for high-lying levels.

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