

State densities and ionization equilibrium of atoms in dense plasmas

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The semiclassical Bohr-Sommerfeld quantization condition is used to derive an approximate analytical expression for the state density of the hydrogen atom in a dense plasma. An ion-sphere model with an infinitely high potential wall is assumed. The expression leads to a universal curve that spans all values of the electron density. The curve is continuous and smooth over the entire energy range, starting from the hydrogenic state density for low-lying bound states and approaching the plane-wave state density in the high-energy limit of the continuum. The number of bound states is approximately proportional to the inverse of the square root of the electron density. Integration of the state density over the Boltzmann distribution of the electronic energy results in an ionization equilibrium relation, leading to modified Saha's equation. The correction factor for this modified equation is a function of both the electron temperature and the electron density, and is expressed as a universal function of the ion coupling parameter.

I. INTRODUCTION

Recent experimental studies of dense plasmas have stimulated theoretical investigations, where the aim is to interpret the spectroscopic properties of atoms and ions contained in such plasmas. These investigations include calculations of energy levels and Stark broadening of bound states, carried out according to various models.^{1,2} These models range from one-electron central-potential treatments, with or without nonspherical perturbation by other particles in the plasma,³ to many-particle treatments in which electron-electron and electron-ion interactions are explicitly taken into account.⁴ These detailed calculations are, however, restricted to low-lying bound states.

For high-lying bound states, there seem to have been no such detailed calculations. Electrons in these states are loosely bound, and their motion is strongly affected by the presence of plasma electrons and ions. The states having a large electron orbit may even disappear. Low-energy continuum states are also expected to be affected strongly. A consequence of these effects may be described as the continuum lowering,⁵ which has been studied in detail theoretically, especially for a partially ionized hydrogen plasma.⁶ In the conventional theory of plasma spectroscopy, the low-lying bound states are often assumed to be those of an isolated atom, the continuum states are assumed to be the free-electron states, and the ionization limit is lowered because of the changes in the average potential. This approximation is useful for some purposes, but may be too crude for other purposes. This is mainly because the assumption of the free states is invalid even for an atom in a low-density plasma; this assumption is equivalent to neglecting the electron-ion interactions, which would be substantial.

Salient features of the emission spectra from plasmas in the recombining phase or in ionization balance⁷ are the series lines (due to bound-bound transitions) converging to the series limit and the recombination continuum (due to "free"-bound transitions). For a low-density plasma, Stark-broadened lines near the series limit merge with their neighbors,⁸ resulting in a continuumlike spectrum. This "quasicontinuum" connects smoothly to the recombination continuum.⁹ This continuation, especially the smooth change of the intensities, cannot be expressed by the above "continuum-lowering" approximation. In fact, we are unaware of any satisfactory explanation of these features in the literature.

For high-density plasmas, the situation is even more complicated. Weisheit and Shore¹⁰ propose a "transparency window" in the higher members of Lyman series of the neutral hydrogen, and an observation of the transparency window is reported on mercury.¹¹ Höhne and Zimmermann¹² claim that the "window" is a numerical artifact of the calculations of Ref. 10. However, another, recent paper reports an observation of a similar phenomenon.¹³ Thus the question of whether the transparency window exists or not is still unsettled.

These facts suggest that our present understanding of the high-lying bound states and the low-energy continuum states of atoms immersed in a plasma is still at a primitive stage. A reasonable model is needed that is capable of interpreting the features as described above. This model should be based on the fact that, for an isolated atom, various properties of high-lying bound states continue smoothly to those of the continuum states across the ionization limit. Naturally, this model and associated calculations should be consistent over the whole range of energies of atomic states, i.e., from the low-lying bound states to the high-energy continuum states.

Saha's equation, which describes the ionization equilibrium relation for atoms and ions in plasmas, is also based on the conventional approximation in which high-lying bound states of an isolated atom are cut off and the free-electron model is used for the continuum states. A quantity important in discussing Saha's equation is the density of states. In the following we consider the density of states of hydrogen in a plasma consisting of neutral hydrogen atoms, protons, and electrons.

We start our discussion with an isolated atom. An electron in a bound state (with an energy $E < 0$) is bound by the Coulomb interaction with a proton. The density of states per unit energy interval is that of the hydrogen atom:

$$g_H(E/R) = |E/R|^{-5/2} \quad (E < 0), \quad (1)$$

where $R (=13.6 \text{ eV})$ is the Rydberg unit. For the free electrons ($E > 0$), the state density is expressed as

$$g_F(E/R) = (E/R)^{1/2} / (2\pi^2 n_e a_0^3) \quad (E > 0), \quad (2)$$

where a_0 is the Bohr radius, and n_e the number density of free electrons.

As shown in Fig. 1, the state density $g_H(E/R)$ diverges as E approaches zero from negative values, whereas $g_F(E/R)$ tends to zero as E approaches zero from positive values. This unphysical discontinuity is due to the inconsistency in the treatments in the positive- and negative-energy regions. In an actual plasma, especially when its particle density is high, the conventional Saha's equation is well known to be invalid; a more elaborate treatment of the state density on both sides of the ionization limit is necessary.

Thermodynamic equilibrium relations, such as Saha's equation, are also important in relating, on the basis of the principle of detailed balance, the rate coefficients for a

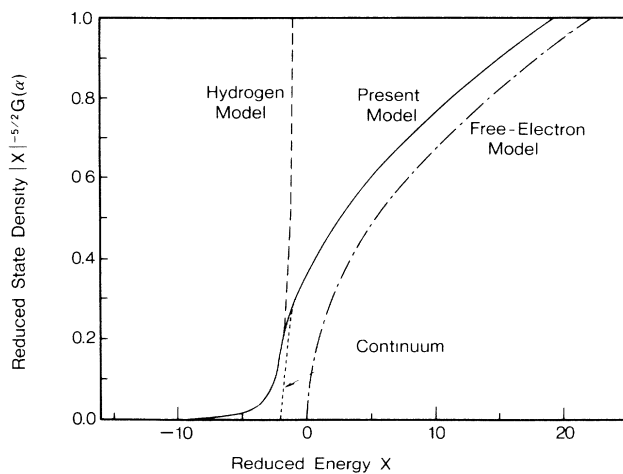


FIG. 1. Reduced density $|X|^{-5/2} G(\alpha) [= (r_i/a_0)^{-5/2} g(E/R)]$ of electronic states as a function of $X [= (E/R)(r_i/a_0)]$; see Sec. III. There are both bound and continuum states in a region $-2 \leq X \leq -1$, and the density of continuum states is separately shown in this region. Also shown are the reduced density of the bound states of the hydrogen atom and that of the free states described by plane waves.

pair of atomic processes that are inverse to each other, e.g., ionization by electron impact and three-body recombination. These rate coefficients are essential for the understanding of the properties of a plasma that deviates from thermodynamic equilibrium. In this respect, we need a reasonable model for the state density that replaces Eqs. (1) and (2). The states of such inequilibrium plasmas may be expressed in terms of a particular population distribution over the state densities over the whole energy range. If the plasma is in thermal equilibrium, this distribution is the Boltzmann distribution at a certain temperature.

As a step toward understanding these properties of plasmas, we present a simple model for the density of states of hydrogen plasmas. We will find that the resultant state density is continuous across the ionization limit, is consistent over the entire energy spectrum, approaches $g_F(E/R)$ at high E , and coincides with $g_H(E/R)$ for low-lying bound states. The ionization equilibrium of dense plasmas is also discussed with use of this state density.

II. MODEL POTENTIAL AND THE BOHR-SOMMERFELD QUANTIZATION CONDITION

We introduce a sphere centered on a proton and with a radius $r_i = (4\pi n_e/3)^{-1/3}$. We refer to this sphere as an ion sphere. It has a volume $1/n_e$, which is the average volume occupied by an unbound electron (and by a proton). The boundary condition on the surface of the ion sphere is often chosen such that no force would act on an electron placed there. In the present paper, however, we adopt a different boundary condition.

We assume that the density of electronic levels in the hydrogen plasma is approximated by the state density of the hydrogen atom confined in an ion sphere, namely, the density of levels held by the electron-proton interaction potential $-e^2/r$ surrounded by an infinitely high potential wall at $r = r_i$. Here, e is the charge of an electron. This model is probably too crude for calculations of particular energy levels. The interest here, however, is not in the shift from a pure hydrogenic level or Stark broadening but in the overall distribution of the level density. The present model should be useful for this purpose. It should be noted that, if the potential inside the infinite wall is zero, the correct free-electron state density per electron, given by Eq. (2), is reproduced, whatever the position of the wall may be. Thus we expect that putting an infinite wall in our model at $r = r_i$ has a weak effect on the density of high-energy continuum states, for which the interaction potential is weak relative to the kinetic energy of the electron. For this reason we will find that the state density in this model approaches $g_F(E/R)$ at high E . The low-lying states that are confined within the ion sphere by the Coulomb potential are unaffected by the wall.

We apply the Bohr-Sommerfeld quantization condition¹⁴:

$$\oint p_r dr = h(n - l - \frac{1}{2}) \quad (3)$$

for the state with a principal quantum number n and an

azimuthal quantum number l , where h is the Planck constant and p_r the radial component of the momentum of the electron. The integral is to be taken over the whole period of the classical motion of the electron, and it is equivalent to twice the integral from the inner turning point $r_<$ to the outer turning point $r_>$. Equation (3) is known to reproduce exactly both the density $g_H(E/R)$ of the quantum states of the hydrogen atom and the density $g_F(E/R)$ of the plane-wave states in a vanishing potential within a finite sphere.

The density dn/dE of states with a given l may be calculated by differentiating Eq. (3) and by noting that $\partial E/\partial p_r$ is the radial velocity v_r , or p_r/m_e , where m_e is the electron mass. It follows that

$$\frac{dn}{dE} = 2(m_e/h) \int_{r_<}^{r_>} p_r^{-1} dr, \quad (4)$$

with

$$p_r = [2m_e(E - V_l)]^{1/2}, \quad (5)$$

where V_l is the effective potential for the partial wave l , i.e., the sum of the Coulomb and centrifugal potentials. Because each (n, l) level is $2(2l+1)$ -fold degenerate (including the spin doublet), the density of states of the hydrogen confined in the ion sphere is the sum of $2(2l+1)dn/dE$ over all possible values of l including zero. This sum is known to be accurately reproduced by the integral over $l + \frac{1}{2}$ from zero to its maximum value, using a semiclassical approximation.

III. DENSITY OF STATES

In the following derivation we use

$$E_0 = e^2/(2r_i) = R/(r_i/a_0) \quad (6a)$$

as the unit of energy, and r_i as the unit of length. We define dimensionless quantities:

$$X = E/E_0 = (E/R)(r_i/a_0), \quad (6b)$$

$$\rho = r/r_i = (r/a_0)/(r_i/a_0), \quad (6c)$$

and

$$\lambda = (l + \frac{1}{2})^2/(r_i/a_0). \quad (6d)$$

The effective potential is

$$V_l/E_0 = -2/\rho + \lambda/\rho^2 \quad (\rho < 1) \quad (7a)$$

and

$$V_l/E_0 = \infty \quad (\rho > 1). \quad (7b)$$

It has a single minimum $-1/\lambda$ at $\rho = \lambda$ and no maximum; the turning points $\rho_<$ and $\rho_>$ depend on both E and λ .

It immediately follows from Eq. (7) that, for $X < -2$, eigenstates exist only for $0 \leq \lambda < |X|^{-1}$, for which $\rho_< < \rho_> < 1$. These eigenstates are identical with the bound states of the free hydrogen atom, because the electron is not affected by the potential wall lying beyond the range of its classical motion. Consequently, the state density for $X < -2$ coincides with $g_H(E/R)$.

For $X \geq -1$, X has a lower value than the potential everywhere in the ion sphere, if $\lambda > X + 2$, and eigenstates exist only for $0 \leq \lambda \leq X + 2$. In this case, the outer turning point is always at the potential wall. If there were no potential wall, the electron in any of these eigenstates would be able to escape into other ion spheres. In this respect, there is no physical distinction between states with a positive energy and those with a negative energy, if $X \geq -1$. Thus all eigenstates in this energy region should be regarded as belonging to the continuum. This may be regarded as continuum lowering due to the existence of the potential wall that simulates the interactions with charged particles outside the ion sphere.

For $-2 \leq X \leq -1$, the outer turning point is at the potential wall if $0 \leq \lambda \leq X + 2$, and the states having an angular momentum in this range should be regarded as belonging to the continuum. In other words, the magnitude of the continuum lowering in our model is $2E_0$.

It should be noted that, in the same energy region $-2 \leq X \leq -1$, there are also bound states, each of which has an angular momentum satisfying $X + 2 < \lambda < |X|^{-1}$. The outer turning point for such a state is inside the ion sphere, and, consequently, the state is identical with a hydrogenic bound state. When $\lambda > |X|^{-1}$, X is lower than the potential minimum and no eigenstates exist.

The density $g(E/R)$ of states in our model, explained in Sec. II, is analytically calculated (see Appendix) to be

$$\begin{aligned} g(E/R) &= g_H(E/R)G(\alpha) \\ &= (r_i/a_0)^{5/2}|X|^{-5/2}G(\alpha), \end{aligned} \quad (8a)$$

with

$$\alpha = X(X + 2), \quad (8b)$$

where

$$\begin{aligned} G(\alpha) &= \pi^{-1} \left[\frac{2}{3}\alpha^{3/2} - \sqrt{\alpha(\alpha+1)} \right. \\ &\quad \left. + \ln(\sqrt{\alpha} + \sqrt{\alpha+1}) \right] \quad \text{for } 0 < X, \end{aligned} \quad (9a)$$

$$\begin{aligned} G(\alpha) &= \pi^{-1} \left[-\frac{2}{3}(-\alpha)^{3/2} - \sqrt{-\alpha(\alpha+1)} \right. \\ &\quad \left. + \sin^{-1}\sqrt{-\alpha} \right] \quad \text{for } -1 \leq X < 0, \end{aligned} \quad (9b)$$

$$G(\alpha) = G_{\text{cont}}(\alpha) + G_{\text{bnd}}(\alpha) \quad \text{for } -2 \leq X < -1, \quad (9c)$$

with

$$\begin{aligned} G_{\text{cont}}(\alpha) &= \pi^{-1} \left[-\frac{2}{3}(-\alpha)^{3/2} + \sqrt{-\alpha(\alpha+1)} \right. \\ &\quad \left. - \sin^{-1}\sqrt{-\alpha - \alpha\pi} \right] \end{aligned} \quad (9d)$$

and

$$G_{\text{bnd}}(\alpha) = \alpha + 1, \quad (9e)$$

and

$$G(\alpha) = 1 \quad \text{for } X < -2. \quad (9f)$$

The leading term in the asymptotic form

$$|X|^{-5/2}G(\alpha) = \frac{2}{3\pi}X^{1/2} \left[1 + \frac{3}{2}X^{-1} + O(X^{-2}) \right] \quad (10)$$

for large X that follows from Eq. (9a) is consistent with Eq. (2) for the free states. This is to be expected since the Coulomb potential has a weaker effect for a larger kinetic

energy. Equations (9a) and (9b) both take the form

$$|X|^{-5/2}G(\alpha) = \frac{4\sqrt{2}}{5\pi} \left[1 + \frac{5}{28}X - \frac{5}{288}X^2 + O(X^3) \right] \quad (11a)$$

near $X=0$. From this expansion and similar expansions near $X=-1$ and -2 , it follows that the state density given by Eq. (8a) is continuous and smooth (with a continuous first derivative) across $X=0$, $X=-1$, and $X=-2$, and over the entire energy spectrum. Also, the state density in our model is a monotonically increasing function of energy. The continuum part of the state density rises linearly from zero at $X=-2$:

$$|X|^{-5/2}G_{\text{cont}}(\alpha) = 2^{-3/2}(X+2) \left[1 - \frac{4\sqrt{2}}{3\pi}(X+2)^{1/2} + O(X+2) \right]. \quad (11b)$$

Figure 1 compares the reduced density $|X|^{-5/2}G(\alpha)$ of states as a function of X with the hydrogenic and free-electron counterparts. The figure also distinguishes the continuum part from the bound-state part; the former is seen to be roughly approximated by $(2/3\pi)(X+2)^{1/2}$, or the free-electron density shifted to the left by two units of X due to the continuum lowering. This has a bearing on a simple modification to Saha's equation, to be discussed in Sec. IV.

Figure 2 shows the density of states $g(E/R)$ for

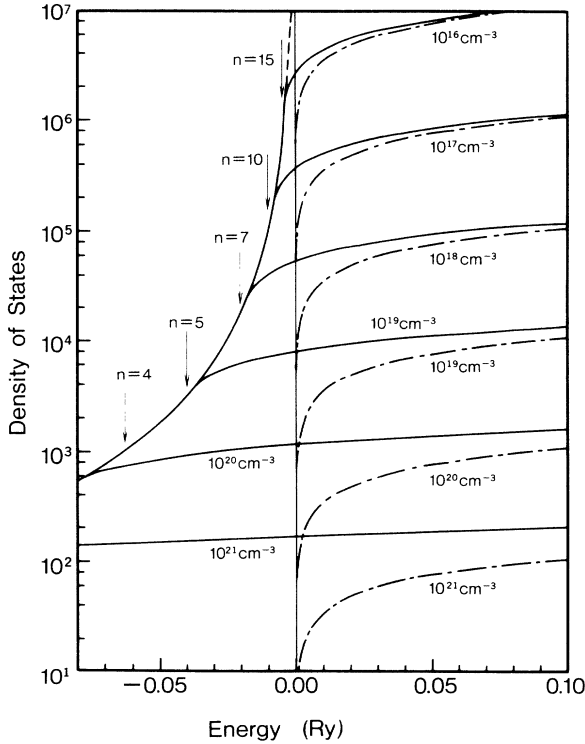


FIG. 2. Density $g(E/R)$ of states (solid curve) for several values of the electron density n_e (attached to each curve) compared with the densities of hydrogenic (dashed curve merging into a solid curve) and free (dash-dotted curve) states. An arrow indicates the position of the hydrogenic levels with a principal quantum number n .

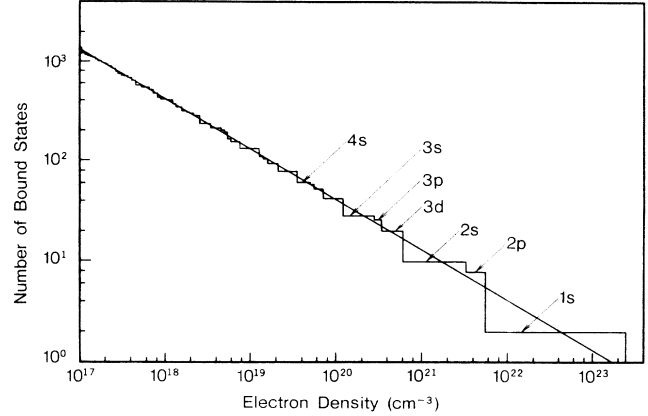


FIG. 3. Number of bound states of the hydrogen atom in a dense plasma, plotted against the electron density n_e . The straight line represents Eq. (13).

several values of the electron density n_e . This figure clearly illustrates that the deviation from $g_H(E/R)$ and $g_F(E/R)$ is larger for the higher values of n_e . The point where the state density starts to deviate from the hydrogenic state density may be calculated from $X=-2$ as

$$E/R = -2/(r_i/a_0) = -(32\pi n_e a_0^3/3)^{1/3}, \quad (12a)$$

or

$$n_* = (2.0 \times 10^{23} \text{ cm}^{-3}/n_e)^{1/6}. \quad (12b)$$

Thus the principal quantum number n_* at the point of deviation is 10 for $n_e \approx 2 \times 10^{17} \text{ cm}^{-3}$, 5 for $1 \times 10^{19} \text{ cm}^{-3}$, 2 for $3 \times 10^{21} \text{ cm}^{-3}$, and 1 for $2 \times 10^{23} \text{ cm}^{-3}$.

The integral of the density of bound states determined by Eqs. (8a), (9e), and (9f) leads to the number N_{bnd} of bound states, including all degenerate states. Thus we have

$$N_{\text{bnd}} = (6\sqrt{2}-8)/(3\pi n_e a_0^3)^{1/2} = (1.7 \times 10^{23} \text{ cm}^{-3}/n_e)^{1/2} \quad (13)$$

for $n_e \ll 10^{23} \text{ cm}^{-3}$. In fact, this number changes discontinuously with n_e . Thus, for the higher electron densities (or smaller N_{bnd}), it is necessary to count the number of bound states rather than to integrate the state density. For extremely large n_e ($n_e > 2.5 \times 10^{23} \text{ cm}^{-3}$), there is no bound state. As n_e decreases, N_{bnd} increases stepwise; $N_{\text{bnd}}=2, 8, 10, 20, 26$, etc., as the levels $1s, 2p, 2s, 3d, 3p$, etc., become bound, i.e., as r_i/a_0 exceeds $1 + \frac{1}{2}\sqrt{3}$, $4 + \sqrt{7}$, $4 + \sqrt{15}$, $9 + \frac{3}{2}\sqrt{11}$, $\frac{9}{2}(2 + \sqrt{3})$, etc. The result given by this step function is compared with the approximate formula (13) in Fig. 3.

IV. IONIZATION EQUILIBRIUM

As an application of the state densities derived in Sec. III, we discuss the thermodynamic equilibrium relation for a plasma at a temperature T . We assume that the electrons in the plasma occupy eigenstates according to the Boltzmann distribution. The integral of this distribu-

tion over the continuum gives the number density n_i of the hydrogen ions. The integral or, more accurately, the sum over the bound-state spectrum gives the number density n_0 of the neutral hydrogen atoms. For the hydrogen plasma, the charge-neutrality condition requires that $n_i = n_e$.

The simplest approximation would be to use the free-electron model, described by Eq. (2), for the continuum spectrum and the hydrogenic model, described by Eq. (1), for the bound-state spectrum. Then it follows that $n_0 = 2N_S\sigma(T)$, where N_S is the normalization constant for the Boltzmann distribution, and where $2\sigma(T)$ is the partition function, i.e.,

$$\sigma(T) = \sum_s s^2 \exp\left[\frac{R/s^2}{k_B T}\right]; \quad (14)$$

k_B is the Boltzmann constant. It also follows that

$$\begin{aligned} n_i &= n_e \\ &= N_S \int_0^\infty g_F \left[\frac{E}{R}\right] \exp\left[-\frac{E}{k_B T}\right] d\left[\frac{E}{R}\right] \\ &= N_S \left[\frac{3}{4\pi a_0^3 n_e}\right]^{1/2} \int_0^\infty \frac{2}{3\pi} \sqrt{X} \exp\left[-\frac{\Gamma X}{2}\right] dX \\ &= 2N_S \Lambda^{-3} / n_e, \end{aligned} \quad (15)$$

where Λ is the thermal de Broglie wavelength of free electrons:

$$\Lambda = h / \sqrt{2\pi m_e k_B T}. \quad (16)$$

The quantity Γ in Eq. (15) is the so-called ion-coupling parameter, which is the ratio of the representative Coulomb energy e^2/r_i ($=2E_0$) to the kinetic energy $k_B T$. Saha's equation,

$$n_0 / (n_i n_e) = \Lambda^3 \sigma(T), \quad (17)$$

follows from Eq. (15).¹

The partition function (14) becomes infinite if the summation is taken over all the bound hydrogenic levels. In view of the continuum lowering, however, the summation should be terminated somewhere. At low temperatures, the partition function hardly depends on the cutoff principal quantum number, unless it is unreasonably large; only the ground state ($s=1$) contributes significantly to $\sigma(T)$ at low temperatures. At higher temperatures and for more accurate treatments of higher energy levels, various methods have been proposed to modify the partition function.¹

According to the arguments in Sec. III, the continuum part of the spectrum in our model is given by Eqs. (9a), (9b), and (9d), and the bound-spectrum part is given by Eqs. (9e) and (9f). Because all the bound states are hydrogenic states, and because the contribution to $\sigma(T)$ from high-lying states is negligible at low temperatures, the neutral density n_0 is nearly the same (at low T) as in Saha's equation to within the normalization constant N_B for the Boltzmann distribution. However, the ion density n_i ,

$$\begin{aligned} n_i &= n_e \\ &= N_B \int_{\text{conti}} g \left[\frac{E}{R}\right] \exp\left[-\frac{E}{k_B T}\right] d\left[\frac{E}{R}\right] \\ &= N_B \left[\frac{3}{4\pi a_0^3 n_e}\right]^{1/2} \int_{-2}^\infty [|X|^{-5/2} G(\alpha)] \\ &\quad \times \exp(-\Gamma X/2) dX, \end{aligned} \quad (18)$$

which is the integral of the Boltzmann distribution only over the continuum, may change drastically from the free-electron case. The correction factor Θ , defined by

$$n_0 / (n_i n_e) = \Theta \Lambda^3 \sigma(T), \quad (19)$$

is the ratio of $(n_i n_e)$ for Saha's equation to that in our model renormalized by N_B . Therefore its inverse may be calculated from

$$\begin{aligned} \Theta^{-1} &= N_B^{-1} \frac{n_i n_e}{2\Lambda^{-3}} \\ &= 3\sqrt{\pi} (\Gamma/2)^{3/2} \int_{-2}^\infty [|X|^{-5/2} G(\alpha)] e^{-\Gamma X/2} dX. \end{aligned} \quad (20)$$

The correction factor depends on both n_e and T , but is a function only of Γ .

The low- and high- Γ behavior of Eq. (20) may be easily studied. First, for small values of Γ , Eq. (20) has a dominant contribution from the integral over large values of X . Therefore the expansion (10) may be substituted into Eq. (20). This leads to a correction factor:

$$\Theta = 1 - \frac{3}{2}\Gamma + O(\Gamma^{3/2}) \quad (21)$$

for small Γ . Retention of only the leading term in Eq. (10), which is equivalent to the assumption of the free-electron model, reproduces Saha's equation $\Theta=1$ as it should. Second, for large Γ , the contribution from $X \simeq -2$ is dominant. Therefore the expansion (11b) may be used in Eq. (20), and the variable of integration may be changed from X to $X+2$. This factors out an exponentially growing factor, and Θ contains an exponentially decreasing factor as

$$\Theta = \frac{2}{3} \left[\frac{\Gamma}{\pi}\right]^{1/2} e^{-\Gamma} \left[1 + \frac{2}{\sqrt{\pi}} \Gamma^{-1/2} + O(\Gamma^{-1})\right]. \quad (22)$$

Figure 4 shows the correction factor as a function of Γ and corroborates the low- and high- Γ forms (21) and (22). Figure 5 compares, for various temperatures, the correction factor as a function of n_e with that obtained by a quantum-statistical method given in Ref. 1.

A simple phenomenological way of correcting Saha's equation for the effect of continuum lowering by ΔE is to replace the ionization potential R/s^2 in Eq. (14) by $R/s^2 - \Delta E$. This introduces an extra factor, $\exp(-\Delta E/k_B T)$, into Eq. (14), as long as the contribution to $\sigma(T)$ from high-lying bound states is negligible. If the free-electron state density (2) is shifted to lower energies by ΔE , the integral of Eq. (15) is unchanged. Therefore the correction factor Θ is $\exp(-\Delta E/k_B T)$. Since

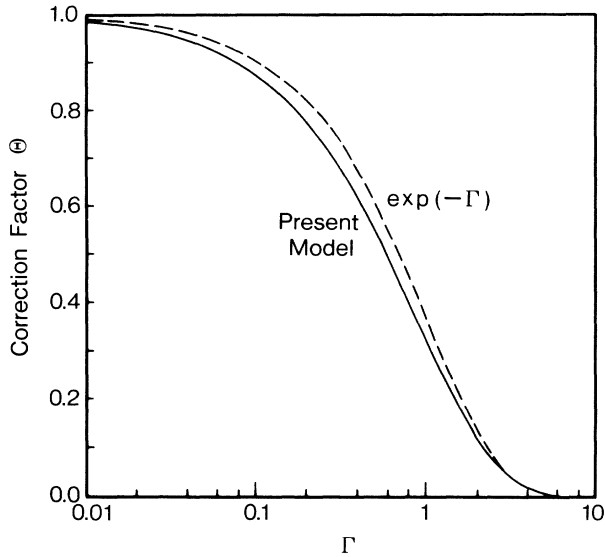


FIG. 4. Universal curve for the factor Θ , defined in Eq. (19), to correct Saha's equation. $\Gamma = (2R/k_B T)(a_0/r_i)$.

$\Delta E = 2E_0$ (or $\Delta X = 2$) in the present model, this phenomenological correction factor equals $\exp(-\Gamma)$ and corresponds to a shifted reduced density $(2/3\pi)\sqrt{X+2}$ for free electrons. Figure 4 shows that this simple approximation largely accounts for the ionization equilibrium in our model. This is consistent with the observation made in Sec. III that the shifted free-electron state density roughly approximates the state density predicted by the model.

It should be noted that, at high temperatures, not only the continuum contribution is corrected by Θ , but the partition function may also be modified.

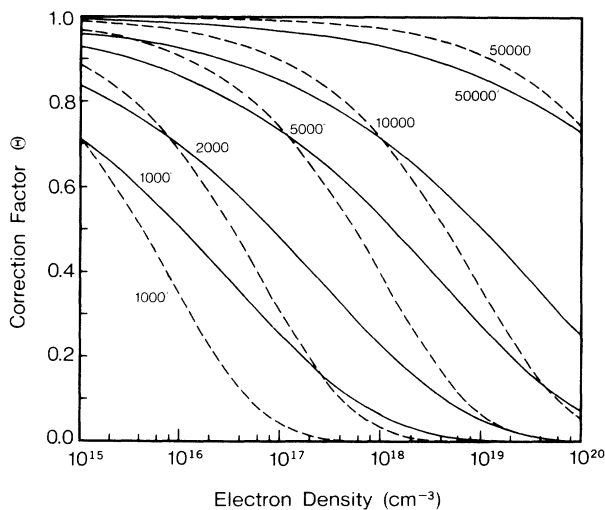


FIG. 5. The factor Θ that corrects Saha's equation (solid curves) as a function of the electron density n_e for several values of the plasma temperature. The dashed curves are the results of the quantum-statistical method of Ref. 1.

V. DISCUSSION

In the model of this paper, the potential field that an electron feels takes a value $-2E_0$ at the boundary of an ion sphere, beyond which the potential field of another ion sphere is lower than $-2E_0$. This is the physical reason for the continuum lowering by $2E_0$ explained in Sec. III. (Bound states exist even above $-2E_0$ depending on the angular momentum, because of the centrifugal barrier.) In other words, the continuum lowering in our model is a result of the lowering of the potential field because of the interaction of an electron with the charged particles other than that proton with which the electron interacts dominantly. The ion-sphere model is often used in the literature with a boundary condition $dV/dr=0$ on the surface of the sphere. In this case, the magnitude of the continuum lowering is E_0 .

Inglis and Teller⁸ (IT) applied the first-order perturbation theory to the Stark shift of the hydrogenic levels due to the field of charged particles in the hydrogen plasma. When the maximum displacement of a level n is larger than half the level spacing, the lines with adjacent n merge into one another, and a quasicontinuum of lines is observed. Assuming that this is the origin of the continuum lowering, they calculated the n value of the highest bound states to be

$$n_*^{IT} = (1.8 \times 10^{23} \text{ cm}^{-3}/n_e)^{1/7.5}. \quad (23)$$

This is to be compared with n_* of Eq. (12b) in our model; note that the point of deviation from the hydrogenic state density gives the continuum lowering in our model. The ratio $r_* = n_*/n_*^{IT}$ is 1.6 for $n_e = 10^{17} \text{ cm}^{-3}$, 1.4 for $n_e = 10^{19} \text{ cm}^{-3}$, 1.2 for $n_e = 10^{21} \text{ cm}^{-3}$, and 1.0 for $n_e = 10^{23} \text{ cm}^{-3}$. The corresponding ratio of the magnitudes of continuum lowering is r_*^{-2} . In the ion-sphere model with a boundary condition $dV/dr=0$ on the surface, the value of n_* is $\sqrt{2}$ times Eq. (12b).

The ion-sphere model is often considered to be a reasonable approximation for strong-coupling plasmas for which the ion-coupling parameter Γ is larger than one. However, the ionization equilibrium derived from the present model appears, in fact, to be reliable, even for weak-coupling plasmas, as is evident from Eq. (21) and Figs. 4 and 5. This result stems from the correct high-energy behavior (10) of the density of states, which is a consequence of the fact about the density of states in the ion-sphere model explained in the second paragraph in Sec. II.

The notion of the density of states applies only to the continuum or quasicontinuum of states by definition. Therefore, naturally, the model of this paper is inaccurate for bound-state spectra with a small number of bound states and, hence, for bound-state spectra for very high electron densities n_e , e.g., close to 10^{23} cm^{-3} .

One of the more accurate methods of computing the ground and low-lying excited states of atoms in plasmas with high n_e is used in Ref. 4. It reports calculations of low-lying energy levels of systems consisting of many atoms in various crystal-cell-like fixed configurations. The tightly bound ground state is found to form a quasi-

molecular orbital in high-density plasmas. By contrast, the present paper deals with the density of states over a wide range of energy spectra, including high-lying bound levels and continua, to which no reliable consistent computational methods appear to have been applied in the literature. Our interest is in the global structure of the density of states, rather than a detailed knowledge of a small number of particular states. For this reason we have paid little attention to the ground and a few excited states, except in the study of the number N_{bnd} of bound states, in which N_{bnd} has been discussed up to high n_e for clarifying the general behavior as a function of n_e .

In conclusion we note that the simple model presented in this paper results in reasonably accurate density of states and ionization equilibrium. Because of its simplicity and the scaling relations, the model should be useful in many practical applications. In the discussion on the modification of Saha's equation, only the correction Θ for the modification of the continuum spectrum has been considered. If the (low-lying) bound levels are shifted to a great extent, or if the plasma temperature T is very high, the partition function $\sigma(T)$ also needs to be modified accordingly.

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APPENDIX

Equations (8) and (9) in the text will be derived here. As explained in Sec. II, the density $g(E/R)$ of states in our approximation is

$$g(E/R) = \int \left[2(2l+1)R \frac{dn}{dE} \right] d\left(l + \frac{1}{2}\right), \quad (\text{A1})$$

where the range of the integration over $l + \frac{1}{2}$ is from zero to the maximum physically allowed value. Equation (A1) may be rewritten as

$$g(E/R) = \left[\frac{r_l}{a_0} \right]^{5/2} \frac{1}{\pi} \int I(\lambda, X) d\lambda, \quad (\text{A2})$$

in terms of the reduced quantities defined in Sec. III, where

$$I(\lambda, X) = \int_{\rho_<}^{\rho_>} \rho (X\rho^2 + 2\rho - \lambda)^{-1/2} d\rho \quad (\text{A3})$$

according to Eqs. (4), (5), and (7) in the text. The smaller turning point is

$$\rho_< = X^{-1}[(1+X\lambda)^{1/2} - 1] \quad (\text{A4})$$

for $X \neq 0$, and the limiting value $\lambda/2$ is to be used for $X = 0$. The greater turning point is

$$\rho_> = 1 \quad \text{for } X \geq 0, \quad (\text{A5a})$$

and

$$\rho_> = \min[1, (-X)^{-1}[(1+X\lambda)^{1/2} + 1]] \quad \text{for } X < 0. \quad (\text{A5b})$$

The use of standard integral formulas leads to the following equations:

$$I(\lambda, X) = X^{-1}(X+2-\lambda)^{1/2} + X^{-3/2} \times \ln \left[\frac{(1+X\lambda)^{1/2}}{X+1+[X(X+2-\lambda)]^{1/2}} \right] \quad \text{for } X > 0, \quad (\text{A6a})$$

$$I(\lambda, X) = \frac{1}{3}(1+\lambda)(2-\lambda)^{1/2} \quad \text{for } X = 0, \quad (\text{A6b})$$

$$I(\lambda, X) = X^{-1}(X+2-\lambda)^{1/2} + |X|^{-3/2} \times \left[\frac{\pi}{2} - \sin^{-1} \left[\frac{X+1}{(1+X\lambda)^{1/2}} \right] \right] \quad \text{for } X < 0 \text{ and } \rho_> = 1, \quad (\text{A6c})$$

$$I(\lambda, X) = \pi |X|^{-3/2} \quad \text{for } X < 0 \text{ and } \rho_> < 1. \quad (\text{A6d})$$

The integral $I(\lambda, X)$ takes different forms depending on whether X is positive or negative. Also, the upper limit λ_{max} of the integration over λ and the turning point $\rho_>$ differ depending on the value of X . Therefore the whole region of X is divided into four: (a) $X < -2$, (b) $-2 \leq X < -1$, (c) $-1 \leq X < 0$, and (d) $0 \leq X$. λ_{max} and $\rho_>$ in each region are discussed in Sec. III: $0 \leq \lambda \leq |X|^{-1}$ and $\rho_> < 1$ in region (a), $0 \leq \lambda \leq X+2$ and $\rho_> = 1$ for the continuum in region (b), $X+2 \leq \lambda \leq |X|^{-1}$ and $\rho_> < 1$ for the bound states in region (b), and $0 \leq \lambda \leq X+2$ and $\rho_> = 1$ in regions (c) and (d). The integration of $I(\lambda, X)$ over λ in each region of X is straightforward by use of standard integral formulas, and Eqs. (8) and (9) may be derived easily.

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