Continuous Free-Electron State-Density Modeling Based on Plasma Microfield

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Following the atomic model based on the microfield in a plasma for bound states [Astrophysical Journal **532**, 670 (2000)], I have considered an atomic modeling for computing the free-electron state-density based on the plasma microfield. In the atomic model based on the plasma microfield, it is considered that an ion in plasma is immersed in a uniform electric field that is the contribution of field values averaged over the other ions in the plasma. It has been expected a modeling for the free-state density consistent with its bound state, because the resulting free-state densities by the simple atomic model based on the plasma microfield has been found to be invalid. In this study, I have obtained a physically appropriate free-state density under the assumption that the large electric field component can be considered to exist due to the electric field originating from the nearest neighboring ion and the resulting potential around the ion shows mirror symmetry about the saddle point. The resulting state density is consistent with the experimental results. The inclusion of the free-state density has caused a slight deviation in the values of the average ionization degree of hydrogenic plasmas.

1. Introduction

Final objective of this study is finding a method to compute the degree of ionization of plasma, which is essentially the analysis of the atomic processes occurring in plasma, based on the plasma microfield. First, I reexamine the conventional method to compute the degree of the ionization of plasmas and show the importance of the state density modeling to the resulting values of the average ionization degree.

In the state of local thermodynamic equilibrium (LTE), the ratio of the product of the number density of the $(Z + 1)$-charged ion N_{Z+1}, and that of the electron $N_e(E)$ of its energy E, to that of the combined Z-charged ion N_Z, is determined by the ratio of the statistical weights of the states of the $(Z + 1)$-charged ion U_{Z+1} to that of the Z-charged ion U_Z, the Boltzmann factor between the two states as given by $\exp(-(E + I_p)/k_B T_e)$, and the number of electron states in free space per unit volume $2(4\pi p^2/h^3)dp$, i.e.,

$$\frac{N_{Z+1}N_e(E)}{N_Z} = \frac{U_{Z+1}}{U_Z} \exp\left(-\frac{E + I_p}{k_B T_e}\right) 2\frac{4\pi p^2}{h^3} dp. \quad (1)$$

In the expression involving the Boltzmann factor, I_p, k_B, and T_e denote the ionization potential from the Z-charged to the $(Z + 1)$-charged state, the Boltzmann constant, and the electron temperature, respectively. In the expression involving the number of electron states, h denotes Planck's constant. With respect to the energy of the free electron

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and its momentum p, the expression $E = p^2/2m_e$ is satisfied, and here, m_e denotes the mass of the electron. Translating the free electron's momentum to its equivalent energy and integrating Eq. (1) over the energy range of the free electron for $E > 0$, we obtain

$$\frac{N_{Z+1}N_e}{N_Z} = \frac{U_{Z+1}}{U_Z} \exp\left(-\frac{I_p}{k_B T_e}\right) \frac{8\pi \sqrt{2m_e^3}}{h^3}$$

$$\times \int_0^\infty \sqrt{E} \exp\left(-\frac{E}{k_B T_e}\right) dE$$

$$= \frac{U_{Z+1}}{U_Z} \exp\left(-\frac{I_p}{k_B T_e}\right) 2\left(\frac{2\pi m_e k_B T_e}{h^2}\right)^{3/2}. \quad (2)$$

This equation is called the Saha-Boltzmann equation. Applying the equation to various ionic species including their excited states in plasma, we can compute the population of all ionic species in the plasma along with the average ionization degree obtained by $Z_{av} = N_e/N_0$ from this computed population, where N_0 is the total number density of ion and atom defined by $\sum N_Z$.

Practically, we need to determine the number of bound states when we apply the Saha-Boltzmann equation for realistic plasmas. For the case of hydrogenic plasmas, Fig. 1 shows one of the difficulties arising out of the conventionally used simple model in which the bound states exist up to a fixed maximum principal quantum number. The contours for an average ionization degree of 0.5 are plotted for three cases in which the maximum principal quantum numbers of the considered bound states are $n = 5$, 10, and
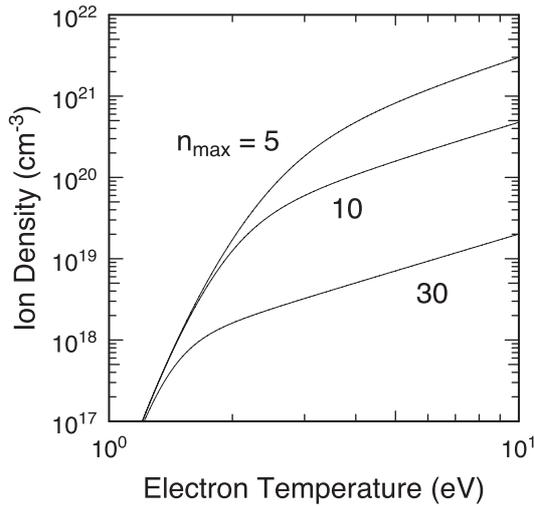
Fig. 1 Contours of average ionization degree are 0.5 of hydrogenic plasmas. The maximum principal quantum numbers of the considered bound states are $n = 5$, 10, and 30.

30. From Fig. 1, it can be observed that the plasma density and its temperature for an average ionization degree of 0.5 varies depending on the maximum principal quantum number of the bound state in the atomic process model. In other words, the plasma density and its temperature for an average ionization degree of 0.5 can be varied by changing the maximum principal quantum number.

In order to address this ambiguity, Nishikawa has suggested a simple analytical expression that allows for the counting of the number of bound states based on the plasma microfield [1]. In the model, hydrogenic ions are assumed to be immersed in a statistically distributed uniform electric field, i.e., the microfield in the plasma. As a result, the potential profile around the ion in plasma is given by the superposition of the ion's Coulomb potential $Z_a e/4\pi\epsilon_0 r$ and the potential due to the uniform external field F; here, Z_a, e, and ϵ_0 denote the nuclear charge of the ion, the elementary charge, and the permittivity of free space, respectively. The hydrogenic ion has a bound state whose energy is given by $-m_e e^4 Z_a^2/8\epsilon_0^2 h^2 n^2$, and this energy is assumed to be unchanging even in the external electric field. In this case, the potential distribution around the ion shows a saddle point. The height of the saddle point varies as the function of the strength of the uniform external electric field. I determine that the electronic state is that of a free electron for energies above this saddle point and that the energy values below the saddle point indicate bound states. Although we now know this is to be quantum mechanically false, this picture can still provide a convenient basis for further improved treatment. From the above assumption, the threshold electric field till which the bound state n exists is given as

$$F_n^c = \frac{\pi m_e^2 e^5 Z_a^3}{64\epsilon_0^3 h^4 n^4}. \tag{3}$$

Although a minor correction factor may be required in the equation, its contribution of determining the threshold principal quantum number n from the electric field F_n^c is expected to be of the order of the one fourth power of the factor. The probability that the bound state n exists is given by the expression

$$w_n = \int_0^{F_n^c} \mathrm{d}F\, P(F), \tag{4}$$

where $P(F)$ represents the distribution function of the microfield. Using the Holtsmark field, given as

$$H(\beta) = F_0 W(F) = \frac{2}{\pi}\beta \int_0^\infty x\exp[-x^{3/2}]\sin(\beta x)\,\mathrm{d}x, \tag{5}$$

as the statistically distributed uniform microfield F, we can compute Eq. (4), where $\beta = F/F_0$, as

$$F_0 = 2\pi\left(\frac{4N_p}{15}\right)^{2/3}\frac{Z_p e}{4\pi\epsilon_0}, \tag{6}$$

where N_p and Z_p denote the number density and the charge state of the perturbing ion, respectively. The term F_0 is called the Holtsmark normal field strength [2]. The Holtsmark field is obtained by summing up the contribution of the electric field from evenly spread ions over space, i.e., the Coulomb interaction between two ions is neglected. Under certain circumstances where the kinetic energy of ions is considerably larger than that of the interaction, the field distribution given by the Holtsmark field becomes appropriate. The simple expression for the probability that the bound state exists, as derived in Ref. [1], is obtained by using the approximation that $H(\beta) \sim 4\beta^2/3\pi$ near $\beta = 0$. It must be noted that given by the equations used in Ref. [1] are incorrect. The correct expression for the probability of the state n is given by

$$w_n = \int_0^{F_n^c} \mathrm{d}F P(F) = \frac{5^2 Z_a^9}{2^{17}\pi^4 n^{12} Z_p^3 N_p^2}, \tag{7}$$

i.e., not the 8th power of Z_a but the 9th power of Z_a. For the hydrogenic case, $Z_a = Z_p = 1$.

At any rate, we can compute the average ionization degrees using the reduced statistical weights of the bound states as obtained from Eq. (4) and the state density for a free electron in free space as described in Eq. (2). For the completeness of the atomic process modeling based on the plasma microfield, it is necessary to include the effect of the plasma microfield in the state density modeling for free electron in addition to the bound state. As described in Fig. 1, the values of the average ionization degree are sensitive on the state density modeling. In this study, we attempt to find an appropriate modeling of the state density for a free electron and evaluate the sensitivity on that.

2. State Density for Free Electron based on Plasma Microfield

In the conventional atomic process modeling, the translation of the electron's momentum to its equivalent energy in the free-state density calculations is carried out using the equations $E = p^2/2m_e$ and $2 \cdot 4\pi p^2 \mathrm{d}p/h^3$. In the present modeling, an ion is assumed to be in a potential that is composed of the Coulomb potential of its nucleus and the potential due to the uniform external field. To accommodate this effect, we rewrite the relation between the electron's energy and momentum at (r, θ) in the spherical coordinates inside the ion sphere radius R_0 as

$$\frac{p^2}{2m_e} = E + \frac{1}{4\pi\epsilon_0}\frac{Z_a e^2}{r} + eFr\cos\theta. \tag{8}$$

The ion sphere has a radius R_0 such that

$$\frac{4\pi}{3}R_0{}^3 N_i = 1. \tag{9}$$

The second term on the right hand side of Eq. (8) indicates the contribution of the Coulomb potential of the nucleus and the third term indicates that of the plasma microfield. This relation shows that even if the electron energy is zero, its momentum does not become zero, i.e., the electron has sufficient kinetic energy to overcome the attractive force of the nucleus from the classical point of view. The state density of the free electron including the potential effect is

$$f(E) = \frac{8\pi\sqrt{2m_e{}^3}}{h^3} \int_0^\infty H(\beta)\,\mathrm{d}\beta \int_0^{R_0} 2\pi r^2\,\mathrm{d}r$$
$$\times \int_0^\pi \sin\theta\,\mathrm{d}\theta \sqrt{E + \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r} + eFr\cos\theta}. \tag{10}$$

In the modeling, the free-state density is computed within the ion sphere of radius R_0. Figure 2 shows the free state density of hydrogenic plasma with ion density $N_i = 10^{16}\,\mathrm{cm}^{-3}$ for various values of $\beta_{\max}$. The term $\beta_{\max}$ indicates the maximum value of the integral range of β in Eq. (10). The reduced statistical weights of the bound states have been computed by using Eq. (4), and not by using Eq. (7). For $E \gg 0$, the free state density defined by Eq. (10) asymptotically approaches $8\pi\sqrt{2m_e{}^3 E}/h^3$. The energy is normalized by twice the hydrogenic ionization potential, $2E_{Ry}$. To understand the continuity of the state densities, we show the bound states as a reduced continuous bound state with a statistical weight $2n^2$ spread over the energy range between the next higher state and the next lower state that leads to an area equal to its original statistical weight $2n^2/(E_{n+1/2} - E_{n-1/2})$, i.e., the area below each step in Fig. 2 is equal to $2n^2$. The reduced continuous bound state profile converges to the the asymptotic behavior of the number of bound state below $E = 0$ given by $2^{-3/2}(-E)^{-5/2}$, as calculated by the relation given by Eq. (8) without including the third term. It may be noted that the vertical axis represents the logarithm scale. The
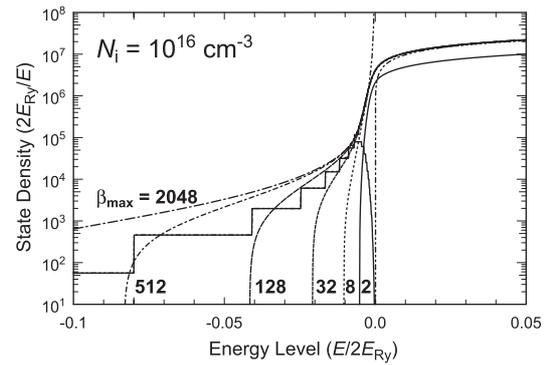
Fig. 2   State densities of free and bound states as obtained by simple atomic model based on plasma microfield for various values of β in Eq. (10). However, the state density of the free electron becomes larger than that of its bound state for the same energy although the values of the free-state density does not diverge.

numbers indicate the principal quantum numbers of the state. Hereafter, we refer to the reduced continuous bound state profile as the reduced bound state density. The two-dot chain curves show the asymptotic bound state density given by $2^{-3/2}(-E)^{-5/2}$, and the state density of electron in free space, $8\sqrt{2\pi m_e{}^3 E}/h^3$, for reference.

From Fig. 2, we can see that the free state density does not become zero at $E = 0$, and it further exists below $E = 0$. However, the free-state density obtained by the simple atomic model based on the microfield is not practically acceptable since the free-state density has been computed as larger than that of a bound electron of the same energy although the values of the state density does not diverge. The effect on the ion-ion correlation is small in the case of the small ion number density values discussed here. The value of Γ, which is the ratio of the potential energy of two ions in the plasma to its temperature, is nearly equal to 0.05 when the temperature of the hydrogenic plasma with ion density $N_i = 10^{16}\,\mathrm{cm}^{-3}$ is $1\,\mathrm{eV}$. Detailed investigations show that the difficulty is induced on the potential far beyond the saddle point inside the ion sphere of radius R_0. Such a large electric field by which the saddle point is sufficiently inside the ion sphere occurs even in the low density plasmas, although the probability is relatively small. The position of the saddle point is given by $r_s = \sqrt{Z_a e/4\pi\epsilon_0\beta F_0}$, while the ion sphere radius is given by Eq. (9). From the equations, it is observed that the saddle point exists within the ion sphere radius when $\beta \geq 5^{2/3}/2\pi^{1/3} \sim 0.998$. This shows that the saddle point is within the ion sphere radius in most situations, and the assumption that the large electric field mostly due to the nearest ion is uniform within the ion sphere radius is inconsistent with the potential measured in real plasmas. In order to overcome this difficulty, we have attempted to compute the free-state density by estimating the contribution of the field values beyond the saddle point assuming the mirror
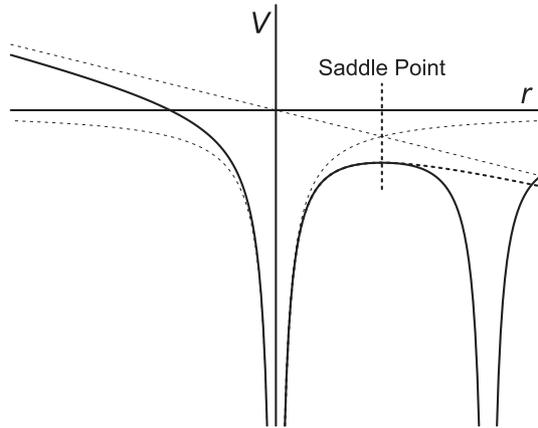
Fig. 3 Schematic figure illustrating potential modification to overcome difficulty arising in simple atomic model including plasma microfield when saddle point of potential is within ion spere radius.
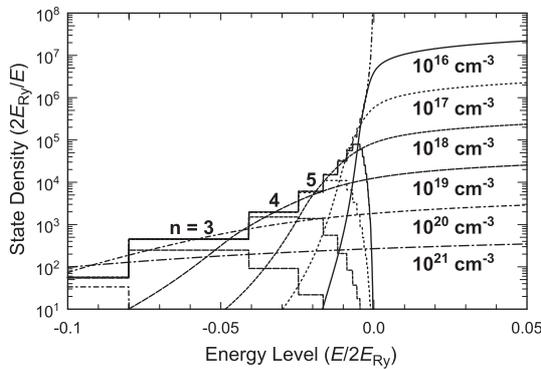
Fig. 4 State density with modification in potential assuming the mirror symmetry with respect to saddle point for various ion number densities ranging from $N_i = 10^{16}\,\text{cm}^{-3}$ to $10^{21}\,\text{cm}^{-3}$ for fully ionized hydrogenic plasmas.

symmetry of the potential with respect to the saddle point. Thus, the potential by which the free-state density is computed is indicated by the solid curve instead of the thick dashed curve in Fig. 3.

Figure 4 shows the energy dependence of the state densities of the free and bound states of hydrogenic plasma by using the above-mentioned potential modeling. The energy dependence curves are plotted for six cases from $N_i = 10^{16}\,\text{cm}^{-3}$ to $10^{21}\,\text{cm}^{-3}$. From Fig. 4, we can understand that the difficulty in the previous computation is induced by the contribution of the potential on the free-state density from far beyond the saddle point, and the free-state densities do not exceed the corresponding asymptotic reduced bound state densities for the same energy.

The quantum states up to the principal quantum number of $n = 8$ are almost completely existing for $N_i = 10^{16}\,\text{cm}^{-3}$. From the state value of $n = 9$, the bound state densities gradually decrease, while the free-state density
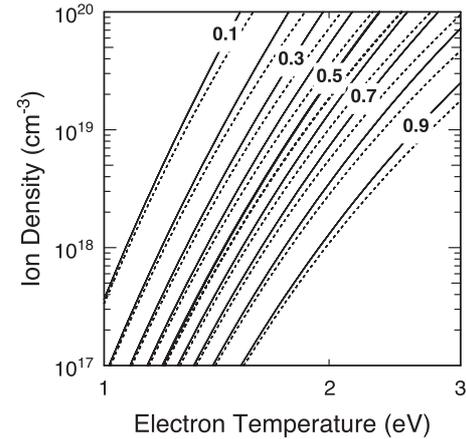
Fig. 5 Average ionization degree of hydrogenic plasma. The potential is assumed to be mirror symmetry with respect to the saddle point.

appears and gradually increases as the principal quantum number becomes larger. Experimentally [3], the bound-bound spectrum from for state values $n = 2$ to 8 in hydrogenic plasma with $N_i = 1.8 \times 10^{16}\,\text{cm}^{-3}$ can be clearly observed, while those for $n \geq 9$ are merged with the free-bound spectrum although the bound-bound spectrum is broadened due to the Stark effect. For $N_i = 9.3 \times 10^{16}\,\text{cm}^{-3}$ in Ref. [3], the bound-bound spectra from for state values of $n = 2$ to 6 can be clearly observed while our model posits bound state existence up to $n = 6$ for $N_i = 10^{17}\,\text{cm}^{-3}$. From our analysis, we might be able to provide a physical meaning for the pseudo-continuum that has been introduced by Däppen [4]. In this light, future studies would be required to examine the state density computation in which the potential distribution and profile of the nearest neighboring ion are actively considered.

Using the model, we can also compute the average ionization degree of various plasmas. In the case of the present model, the free state density $f(E)$ is used instead of $\sqrt{E}$ in Eq. (2), i.e.,

$$\frac{N_{Z+1}N_e}{N_Z} = \frac{U_{Z+1}}{U_Z} \exp\left(-\frac{I_p}{k_B T_e}\right)$$
$$\times \int_{\max(-\frac{e^2 Z}{4\pi\epsilon_0 r} - eFr\cos\theta,\, -2e\sqrt{\frac{eZ_a F}{4\pi\epsilon_0}})}^{\infty} f(E) \exp\left(-\frac{E}{k_B T_e}\right) dE. \tag{11}$$

It is noted that the lower range of the integration on E has been changed to be from 0 to the larger value of just potential at the point, $-e^2 Z/4\pi\epsilon_0 r - eFr\cos\theta$ or potential at the saddle point, $-2e\sqrt{\frac{eZ_a F}{4\pi\epsilon_0}}$ since the state density of which energy is below the value of its saddle point is assumed to be bound in this model. Figure 5 shows the average ionization degree of hydrogenic plasma. The dotted curves in Fig. 5 are the results obtained using Eq. (2), while the solid curves are those obtained by Eq. (11). From Fig. 5, it is observed that the contours including the potential effect in the

free-state density deviate slightly to the lower temperature region since the free-state density exists continuously from the bound state. The deviation is not very large; however, the deviation grows larger as the plasma density increases.

In conclusion, I draw attention to one of the features of the present model in comparison with other models in which the concept of the ion sphere is used [5]. Most atomic models that apply the concept of an ion sphere only consider the plasma effects on the resulting potential in a spherical fashion. Therefore, we sometimes encounter the difficulty of the sudden disappearance of a bound state at a given threshold density when we compute the average ionization degrees over a wide range of plasma density and temperature. Using the present model, we can avoid such difficulties since the bound states gradually decrease as the density increases.

3. Summary

In this study, I have considered an atomic model to compute the free-electron state-density based on the microfield in a plasma. In the atomic modeling based on the plasma microfield, it is considered that an ion in plasma is immersed in a uniform electric field that is the contribution of the field values averaged over the other ions in the plasma. The Holtsmark Field is used to obtain the distribution of the uniform electric field in plasma throughout this study. However, the resulting free-state densities obtained by the simple atomic model are invalid, i.e., the free-state

density becomes larger than those of the bound states. The problem arises from the presence of a large electric field component, although its probability of occurrence is relatively small. A large free-state density is induced on the potential far beyond the saddle point inside the ion sphere radius. If the large electric field component can be considered to exist due to the electric field originating from the nearest neighboring ion, and the resulting potential around the ion is assumed to show mirror symmetry with respect to the saddle point when the nearest neighboring ion is within the ion sphere, the physically appropriate free-state density, which appears when the bound state disappears, can be computed. The resulting state density is consistent with the experimental results. The inclusion of this effect causes a slight deviation in the values of the average ionization degree of hydrogenic plasmas. This model is different from most other former models previously used since the state densities of the free and bound electron are computed using a non-spherical potential profile.

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