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Modeling of the Coulomb interaction between a pair of ions by the nearest neighbor approximation
最近接近似におけるイオン間クーロン相互作用モデル

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A new atomic process model in plasmas based on the nearest neighbor approximation is considered. Using the model, we can evaluate the plasma effect on the free state density although most conventional models do not treat them. In order to show the usefulness of the model, the ability of analyzing the plasma of near and above solid density is indispensable. In this paper, a simple expression introducing the Coulomb interaction between a pair of ions is adopted in the nearest neighbor ion's distribution. The details of the expression introducing the Coulomb interaction and typical results for the hydrogen plasmas are shown.

1. Introduction

I consider building up a new atomic model in plasmas based on the nearest neighbor approximation. In the model, the plasma effect in the atomic process is considered as summation of nearest neighbor ion's contribution from various distances. Most conventional models [1] have treated the effect as the plasma microfield and they do not consider the effect on the free electrons. Using the model, we can evaluate the free state density as well as the bound state density shown in Fig. 1. The basic ideas and typical results of hydrogen plasmas had already published in literature [2].

To demonstrate the usefulness of the new atomic model, applicability of the model for dense plasmas of near and above solid density is indispensable. In the previously presented paper [3], I had suggested a simple consideration of the Coulomb interaction between a pair of two ions. Unfortunately, the expression is not exactly true. In this paper, I reexamined the probability of existing the nearest neighbor ion with considering the Coulomb interaction between a pair of two ions in detail.

2. Coulomb interaction between a pair of ions

I try to include the Coulomb interaction into the probability finding an ion at r as the Boltzmann factor of the ratio of the potential energy between a pair of ions and their kinetic energy. I considered the probability as the following type of expression:

$$g(r) = C\exp\left(-\frac{Z^2e^2}{4\pi\varepsilon_0 r k_B T_i}\right). \qquad (1)$$

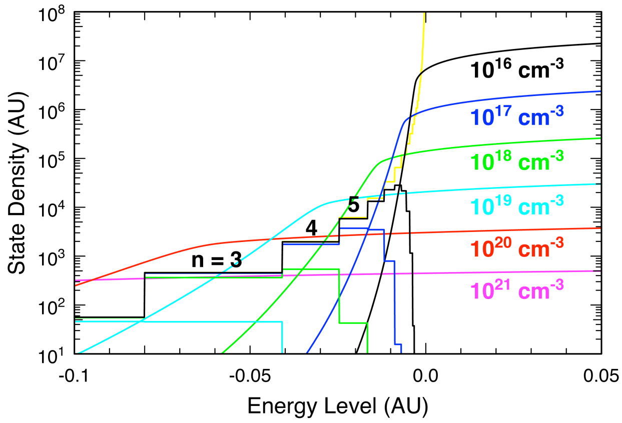

Fig.1 State densities of bound and free electron for various ion number densities in fully ionized hydrogen plasmas, as obtained by an atomic model based on the nearest neighbor approximation.

C is the constant that satisfies

$$\int_0^{R_2} g(r)4\pi r^2\,dr = 1 \qquad (2)$$

where Z, e, and ε_0, k_B, T_i denote the nuclear charge of the ion, the elementary charge, the permittivity of free space, the Boltzmann factor, and the ion temperature, respectively. R_2 is defined by $4\pi R_2^3 N_i / 3 = 2$ where N_i is the ion number density. This attributes that two ions exists in the ion sphere of radius R_2. One is the center of the sphere and the other is the nearest neighbor ion.

The probability that the nearest neighbor ion exists at R can be translated into the probability that there are no ions inside the sphere of radius R and an ion on its surface:

$$\prod_{V_s}\left(1-g\left(r_n\right)\delta V\right)^{4\pi r_n^2\delta r/\delta V}\sum_{S_s} g\left(R\right)\delta S \qquad (3)$$

where V_s and S_s are the volume and surface area of the sphere of radius R. This is mathematical expressed by

$$P\left(R\right)dR=\exp\left(-\int_0^R g\left(r\right)4\pi r^2\,dr\right) g\left(R\right)4\pi R^2 dR \qquad (4)$$

This expression can be found in Salzmann's textbook [4]. The value of definite integrant of the Eq. (4) from 0 to ∞ becomes unity although the corresponding expression shown in Ref. [3] does not become unity.

3. Neutral atom's contribution

Even in the hydrogen plasmas, there are two kinds of particles, i.e., ion and atom. In the following, I only consider hydrogen plasmas. In the case, we have to define two probability functions, $g_i(R)$ = C_i $g(R)$ for ions and $g_n(R)$ for atoms. I assumed there are no bound states if the nearest neighbor atom is located within the distance less than the threshold radius of n = 1. The threshold radius is given by $r_{th} = 8\varepsilon_0 h^2 n^2/\pi m_e e^2 Z$ where h and m_e denote Planck's constant and the mass of the electron, respectively. If the nearest neighbor ion locates outside the threshold radius, the atom has the bound state of its principal quantum number n. (The details are described in Ref. [2].) This means that both become ions if two atoms are located within the threshold radius. Moreover, $g_n(R)$ = C_n is assumed to be uniform because there are less interaction if a part of pair is non-charged atom. In the case including the neutral atom,

$$\int_0^{R_2} g_i\left(r\right)4\pi r^2\,dr+\int_{r_{th},n=1}^{R_2} g_n\left(r\right)4\pi r^2\,dr=1 \qquad (5)$$

is satisfied instead of Eq. (2). Practically, Eq. (5) is solved iteratively with the ion density in the atomic process computation.

4. State densities of free and bound electrons

The probability of the bound state of the hydrogenic ion, of which principal quantum number is n, is given by

$$w_n=\int_{r_{th}}^{\infty}\exp\left\{-\int_0^R\left(g_i\left(r\right)+g_n\left(r\right)\right)4\pi r^2\,dr\right\} \left(g_i\left(R\right)+g_n\left(R\right)\right)4\pi R^2 dR \qquad (6)$$

For the free state, the state density $f(E)$ as a function of the electron's total energy of the potential and kinetic energy is calculated by

$$f\left(E\right)=\frac{8\pi\sqrt{2m_e^3}}{h^3}\left\{\int_0^\infty P_i\left(R\right)dR\int_0^{R_1}2\pi r^2\,dr\int_0^\pi \sin\theta\,d\theta \sqrt{E+\frac{Ze^2}{4\pi\varepsilon_0}\left(\frac{1}{r}+\frac{1}{\sqrt{R^2-2Rr\cos\theta+r^2}}\right)}+\int_0^\infty P_n\left(R\right)dR\int_0^{R_1}2\pi r^2\,dr\,2\sqrt{E+\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{r}}\right\} \qquad (7)$$

using the probability of finding nearest neighbor ion and atom, $P_i(R)$ and $P_n(R)$. I used the relation between the electron's energy and momentum at (r, θ) in the spherical coordinates inside the ion sphere radius R_1 as $4\pi R_0^3 N_i$ / 3 = 1. To accommodate the effect, we rewrite the relation between the electron's energy and momentum as for the ion:

$$\frac{p^2}{2m_e}=E+\frac{Ze^2}{4\pi\varepsilon_0}\left(\frac{1}{r}+\frac{1}{\sqrt{R^2-2rR\cos\theta+r^2}}\right) \qquad (8)$$

and for the atom:

$$\frac{p^2}{2m_e}=E+\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{r}. \qquad (9)$$

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