IPPJ-AM-57

ATOMIC MODELS FOR HOT DENSE PLASMAS

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January 1988

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[†] This work was carried out under the Collaborating Research Program at the Institute of Plasma Physics, Nagoya University, Nagoya.

Contents

Preface

Heavy ions and laser beams of high power densities are the main drivers to produce extremely high temperature and high density plasmas which would eventually lead to the nuclear burning. The studies on hot dense plasmas are particularly important to diagnose the plasma and investigate radiation heating or cooling mechanism in it. Experimental data on atoms in dense plasmas, which have accumulated rapidly, also require the knowledge of fundamental characteristics of atoms immersed in plasma for their analysis. Up to now, many theoretical investigations have been reported on an atom or a few-atom cluster in plasmas. In this article, we are intending to review those studies with a hope of providing new comers with an introduction to those problems. With the maximum effort, however, we have to leave some important aspects of the problem undiscussed. The references given at the end of this article may provide necessary information.

In the introductory section I, a fundamental method of our approach to the atomic states in plasma is stated. This is intended to make our standpoint adopted in succeeding discussions clear and cast the light on the problems which are usually left undiscussed. Many of the readers may feel that atomic models which appear in the succeeding sections do not follow this scenario. However, what we are insisting in this article is nothing but this inconsistency of the conventional theories. Section II deals with a hydrogenic atoms in plasma in terms of classical model potentials. These model potentials introduced in this section are also used in the following sections. we devote section III to the discussion of Thomas Fermi Models at finite temperature because of their simplicity and wide application. Quantal treatments of the problem are discussed in Section IV.

We strict our attention to the atomic models in plasma and do not intend to go into the elementary processes, such as collisional excitation and ionization by electrons, charge transfer process and so on. The quantitative understanding of these mechanisms are now becoming to be an urgent problem for the design of a nuclear fusion reactor. We hope a review article by Karashima et al,$^{1)}$ which is one of the IPP reports, on "Theories of stopping power for heavy particles in hot and dense plasma', will cover a part of these problems.

I Introduction

In general, physical properties of matter can be classified into two categories, i.e., macroscopic and microscopic properties. The microscopic phenomena, such as X-ray emission, absorption, atomic collisions accopmanying charge transfer, ionization and excitation of electrons, are described fairly well, in many cases, by considering a single atom or a small molecule, even though the actual atom or molecule is immersed in continuous media. However, this treatment is inadequate for the calculation of the equation of state, electronic conductivity, and energy and heat flow and so on, because these are concerned with the macroscopic properties of the matter. The same is true for the high density and high temperature plasmas. As is indicated by the title of this article, here we focus mainly upon the microscopic properties of hot dense plasmas based on atomic models.

Suppose a plasma is defined as a medium composed of positive and negative charged particles moving almost freely but still interacting each other and its state is defined only through the macroscopic physical quantities. These quantities, often called plasma parameters, are expressed by the language of statistical mechanics; that is, an average of the operator over the grand cannonical ensamble. Atomic process takes place under the physical condition which is controlled not by the microscopic parameters but by the macroscopic ones. This means that when we study atomic process in plasmas with certain plasma parameters, we should always reduce them into microscpic conditions. On the contrary, if we intend to estimate the thermodynamic properties of the plasma, we need to know eigenstates of the system for the purpose of calculating the partition function or interaction Hamiltonian between almost free particles or quasi-particles and to perform the perturbation expansion. (This statement may sound misleading. We do not necessarily need the eigenstates of a system to calculate a thrmodynamic quantity. Computing a trace of an operator with any infinite Fock space is enough; the result should not depend on the choice of the space. However, since it sometimes turns out to be impossible to calculate the trace with infinite basis, we have to use a finite basis as an approximation. For that purpose, a set of accurate eigenstates should be known. Reference 2 gives a discussion about this point.)

So, the study of atomic properties in hot dense plasmas is important for the two reasons; for the analysis of elementary processes in the plasmas itself and for the basic research of the other properties which can be obtained as a result in statistical averaging.

Now we look at some of the important properties of an atom in plasmas. As a representative example, we start the discussion with an X-ray emission spectra in inertial confinement experiment using high power laser beams. Figure 1 shows a spectrum of silicon atoms in glass a micro balloon observed in the inertial confinement fusion experiment. As is seen in this figure, the observed spectrum usually exhibit sharp emission and absorption lines. The sharpness of these lines suggests that the atoms which radiate these X-rays are in ionic states which are not so much different from free ionic states. Actually, these lines can be, in most cases, assigned easily on the basis of the energy-level diagrams of an isolated highly charged ion. Though the dominant features of the spectrum are similar to that of a free ion, some differences are found from the isolated ion spectrum which are due to the effect of high density and high temperature circumstances. A careful investigaton of the optical spectrum provides us detailed information about the electronic states of the plasma.

The first difference appears in the energy of the lines. This is due to the change in the degree of the electron screening of the ion core charge. The amount of the energy shift corresponds to the plasma density and temperature through this degree. Estimation of the line shift by using the plasma parameters is one of the main purpose of this research.

The second is the lowering of Rydberg series limit. This effect is often called as continuum lowering and is interpreted in the following: when the plasma becomes dense, highly excited states or Rydberg states lose their discrete properties because other neighboring ions come and fall inside the orbital radii of the Rydberg electrons. These orbitals cease to be atomic and

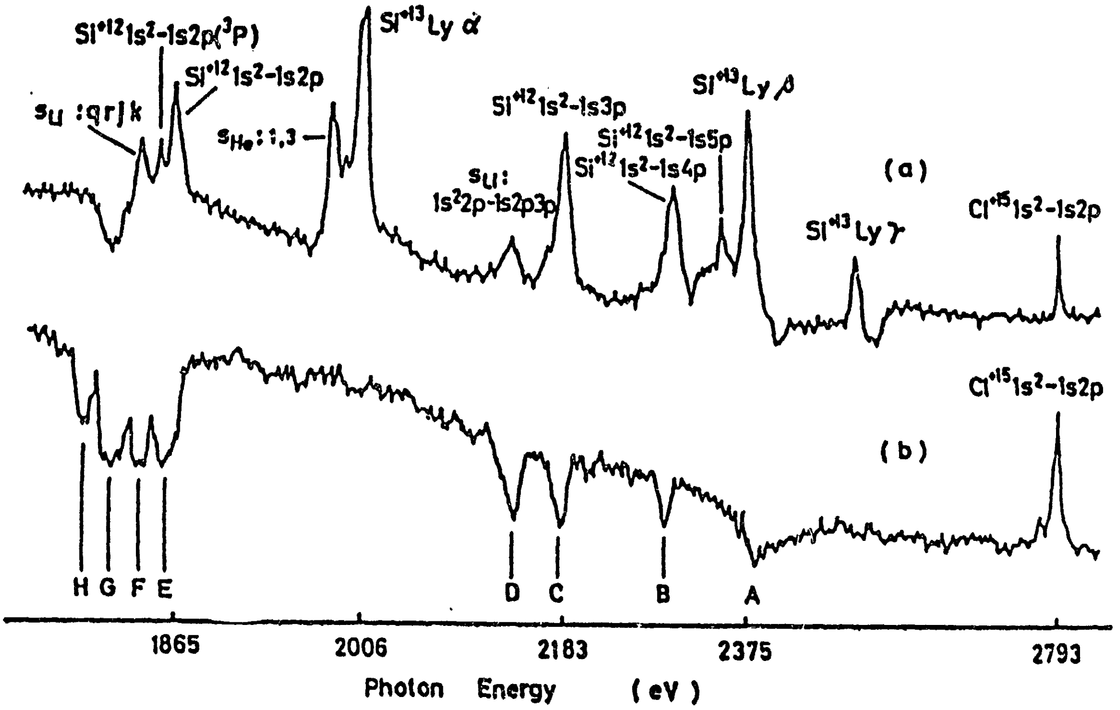

Fig. 1 X-ray spectra of Si ion emitted from glass micro balloons. Maximum compression estimated is 20 g/cm^3 at 200 eV for the spectrum (a) and 50 g/cm^3 at 50 eV for (b) reprinted from N. Miyanaga, Y. Inada and Y. Kato "Annual Report on Laser Fusion Program" JIE. Osaka Univ. 42 (1979).

they are treated as the molecular or band-like orbitals which are realized in the solid state. Accordingly, the peak which corresponds to a transition from these orbitals becomes so broad that the spectrum becomes quasi-continuum. This phenomenum looks as if the ionization limit is lowered. The details will be discussed later.

The third feature found in the spectra is the existence of broad peaks. These broad peaks could result from the convolution of sharp peaks with an instrumental function of rather poor resolution. There is yet another possibility that wavefunctions concerning these transitions depart appreciably from the discrete atomic ones. They may be delocalized orbitals or the band-like orbitals like those in solid state. The Doppler-broadening will enlarge the half width, too. Their analysis is rather complicated. Since a time-resolved observation of the X-ray spectra is very difficult, we can not expect to obtain more detailed information from experiment. At present, we do not know much about these wide peaks. The study of them has just started taking the delocalized or molecular orbitals into consideration.

Anyway these spectra contain the information about how high the plasma temperature is and to what extent atoms in the plasma are ionized. In order to answer these questions, the one-electron energies of initial and final states and the transition probabilities between them should be known. To the first approximation we need only the wavefunctions of electrons which interact with photons. Accordingly, the practical requirement for electronic state in plasma is to obtain a suitable **effective potential** in the Shroedinger equation and boundary condition of wavefunctions.

Here we use a word **effective potential** without any definition. For hydrogenic atoms in a plasma, which will appear in section II, its meaning is rather clear. The effective potential for a core electron is the result of the interaction only between the bound electron in question with other free electrons and surrounding ions. This implies that the state of free electrons and the interactions between ions are not affected much by a slight change of a core state. However, the boundary condition of the wavefunction is not so clear. In the isolated atomic case, the boundary condition of the wavefunction is zero at infinity. Since the atom in question is in plasma, the wavefunction which has a large amplitude at the neighbouring ion is questionable in its reality.

In order to make our problem clear it would be better to start with the general description of the problem.

In hot dense plasma an atom is surrounded by many ions and electrons move rapidly. Therefore, we can not neglect the interactions between the atom and these surrounding ions and electrons. If we try to calculate the atomic states, the motion of ions and electrons should be known; in other word, we need to have the knowledge about the correlation between the atom and ions. For this purpose, electronic states of the atom should be known. Therefore we have to repeat the same procedure without an end. An ideal approach would be to solve the problems of atomic states and of the motion of ions and electrons at the same time. However, since this results in an extremely complicated problem, the motion of the ions are, in many cases, supposed to be solved in advance and represented in a statistical way in the course of the calculation of the atomic problem. This is equivalent with the assumption of separability of nuclear and electron coordinates for the total wavefunction.

Let's write the Hamiltonian of N electrons and M nuclei system,

$$H = -\frac{\hbar^2}{2m_e}\sum_{\nu}\nabla_{\nu}^2 + \frac{1}{2}\sum_{\mu\neq\lambda}\frac{1}{|r_{\mu}-r_{\lambda}|} + [-\frac{\hbar^2}{m_N}\sum_{k}\nabla_k^2 + \frac{1}{2}\sum_{i\neq j}\frac{Z_iZ_j}{|R_i-R_j|}] - \sum_{\nu,k}\frac{Z_k}{r_{\nu}-R_k} \qquad (1-1)$$

where r and R stand the position of electrons and nuclei, respectively. We use Atomic units without otherwise noted. The Shrodinger equation can be written as,

$$i\frac{d\psi(r,R:t)}{dt} = H\Psi(r,R:t) \qquad (1-2)$$

If an appropriate initial or boundary condition is given and the Shroedinger equation can be integrated, then the plasma parameters can be calculated by using the partition function. Since this approach is practically impossible as mentioned above, we assume that the total wave function is separable into wavefunctions of the electron and those of the nuclei, i.e.,

$$\Psi(\mathbf{r},\mathbf{R},t)=\phi(\mathbf{r},t)\Phi(\mathbf{R},t). \qquad (1\text{-}3)$$

Our present problem is not to obtain the motion of nuclei but to calculate the electron wavefunction. In most cases we suppose $\Phi(\mathbf{R},t)$, which represents the motion of nuclei, is known. Removing the terms of the kinetic energies and potential energies between nuclei, the time dependent Hamiltonian for the electron system can be written as

$$H_{el}=-\frac{\hbar^2}{2m_e}\sum_{\nu}\nabla_{\nu}^{2}+\frac{1}{2}\sum_{\lambda\neq\mu}\frac{1}{|r_{\lambda}-r_{\mu}|}-\sum_{\mu,k}\frac{Z_k}{|r_{\mu}-R_k(t)|} \qquad (1\text{-}4)$$

where $\mathbf{R}_k$'s are given by the $\Phi(\mathbf{R},t)$. Here in Eq. 1-4, nuclear coordinates are assumed to be expressed in semi-classical way and are included into the Hamiltonian only parametorically.

Nuclear motion may affect the electronic property. Its contribution depends on the time scale of the process which are considered. For a hydrogen plasma at temperature 10 keV, the average speed of nuclei is about 0.6 a.u.. Since radiation and absorption of photons are usually very fast processes, the time dependence of $\phi(\mathbf{R},t)$ can be considered as static. This corresponds to the assumption that each electron forgets what ion it originally has belonged to. However it is a well known fact that, for processes like charge transfer, collisional excitation and ionization, the motion of electrons with respect to a particular nucleus sometimes plays important roles when the collision velocity is larger than unity.

Apart from the time dependence of $\mathbf{R}(t)$, the Hamiltonian at this stage is that of a familiar multielectron multi-center system. Since this problem itself is an extremely difficult task, we must make some approximation. Three kinds of approximations are commonly used in which one can take the contributions of nuclear potentials into consideration. Since the regularity or periodicity of atomic configuration ($\mathbf{R}_j$) can not be assumed in the plasmas, the first one emphasizes this irregularity or randomness of the atomic configuration. The **Coherent Potential Approximation (CPA)**, which is often applied to the random system such as amorphous, is an efficient approach. Kishimoto and Mima have applied this method to neon plasmas. The second is the method to take the time average of the ionic configurations. Many workers can reduce the potential can be reduced into spherical ones by this method. The **Debye-Huckel, Ion-Sphere**, the **Stewart-Pyatt** models and more elaborate ones are widely used for this purpose. The simplest one is to assume the regularity of the atomic configuration for the plasma even though it is considered rather far from the reality. The **muffin-tin Thomas-Fermi model** and an approach based on **DV-Xα** belong to this group. Theories of the first and the third groups include the features that electrons can move around every ions in plasmas resulting in the binding nature between the ions. However, approaches based on the second group usually neglect this effect.

The contribution form the ions is approximated to be spherical symmetric, then the H_{el} reduces to

$$H_{el} = [-\frac{\hbar^2}{2m}\sum_{\nu}\nabla_{\nu}^2 + V(r)] + \frac{1}{2}\sum_{\lambda\neq\mu}\frac{1}{|r_\lambda - r_\mu|} \tag{1-5}$$

Even in this approximation Hamiltonian is still that of multielectron problem. If all the electrons in the system are assumed to be in bound states and if we do not mind the amount of calculation, there are some possibilities to carry out the integration of the Shroedinger equation. However, it is difficult to calculate an accurate wavefunction of multi-excited state with the present ability of computational method.

To separate the electronic wavefunction into the parts of free electron and bound ones is one of the practical ways, though this gives rise to a new problem: i.e., how many electrons are in the bound states . Under this approximation, the Hamiltonian in question is in the form

$$H_{el'}^{\ bound} = [-\frac{\hbar^2}{2m}\sum_{\nu\in bound}\nabla_{\nu}^2 + V_{eff}(r)] + \frac{1}{2}\sum_{\nu,\lambda,\in bound}\frac{1}{|r_\nu - r_\lambda|} \tag{1-6}$$

The potential $V_{eff}(r)$ in Eq. 1-6 now includes the interaction between the bound and free electrons.

Average Atom model and **Quantum Cell Model** are based on this Hamiltonian or its relativistic form and we solve the Hartree-Fock or Dirac equations. Going into further approximation, we can neglect the shell structure of atoms and molecules. This leads to the idea of the **Thomas-Fermi** or **Quantum-statistical Models.**

Here we summarize the difficulties encountered when we solve the problems of atoms in plasma. First, the motion of surrounding ions can not be taken into account in an ordinary framework of treatment. Second, if ions are considered to be fixed in space, their configuration is random. So, we can not use the familiar idea of the 'unit cell' as in solid state physics. Accompanying to this point, the boundary condition of the wavefunction can not be clearly defined. Third, the system has many ionized electrons. This makes the problem more difficult. We can not distinguish free wavefunction from bound one when Hamiltonian of the system is approximated and the boundary condition can not be definitely stated.

II Classical Model Potentials and Hydrogenic Atoms

Three theoretical models presented in this section treat the motion of positive ions and electrons classically. The first one is the **Debye-Huckel theory** which is valid for high temperature and low density plasma (i.e., the ion-coupling parameter $\Gamma \ll 1$. is the ratio of kinetic energy of ions due to thermal motion to the Coulomb potential between them. If the effective charge of the ions is Z^*, Γ is written as $(eZ)^2/K_bT$). The second model is the **Ion-sphere model.** This model is useful when Γ exceeds unity. The final model is called the **Pyatt-Stewart model.** This reduces to the above two models at the two extremes of Γ. By separating the bound electrons from the free ones, this model lead us to the concept of so-called "continuum lowering".

II-1 Debye-Huckel Model

II-1-A Debye-Huckel Model Potential

Let $n_e(\mathbf{r})$ and $n_i(\mathbf{r})$ $(i=1,2,...N)$, be the number densities of electron and the i-th positive ions of charge Z_i at position **r**. These particles are in thermal equilibrium at temperature **T**.

The electronic potential **V(r)** for an electron around a positive charge Z_0 satisfies the Poisson eq.

$$\nabla^2 V(r) = -4\pi e\left(\sum_i Z_i n_i(r) - n_e(r) + Z_0 \delta(r)\right). \tag{2-1}$$

where $\delta(r)$ stands for the three dimentional delta function.

The charge neutrality condition of the system is written as

$$\sum_i^N Z_i n_i(\infty) = n_e(\infty), \tag{2-2}$$

where $n_i(\infty)$ and $n_e(\infty)$ are the density of the ith ions and electron at infinity, respectively.

At the high temperature limit, both electrons and ions are in Maxwell distribution,

$$\begin{aligned} n_i(\mathrm{r}) &= n_i(\infty)exp(Z_i e V(\mathrm{r})/k_B T), \\ n_e(\mathrm{r}) &= n_e(\infty)exp(-eV(\mathrm{r})/k_B T). \end{aligned} \tag{2-3}$$

If $\beta = 1/(k_B T)$ is small, Eq. (2-3) can be expanded in the form

$$\begin{aligned} n_i(\mathrm{r}) &= n_i(\infty)[1+\beta Z_i e V(\mathrm{r})], \\ n_e(\mathrm{r}) &= n_e(\infty)[1-\beta e V(\mathrm{r})]. \end{aligned} \tag{2-4}$$

By substituting Eq. (2-4) into (2-1), we obtain the Poisson equation for the system,

$$\nabla^2 V(r) = 4\pi e(\sum_i n_i(\infty)\, Z_i - n_e(\infty)) \tag{2-5}$$

$$+ 4\pi e Z_0 \delta(r) - 4\pi e^2(\sum_i Z_i^2 n_i(\infty) + n_e(\infty) V(r)$$

The first term in Eq.(2-5) is zero from the neutrality condition of Eq.(2-2). A relation $n_e(\infty) = \sum_i Z_i(\infty)$ reduces Eq (2-5) into

$$\nabla^2 V(r) = -4\pi\beta e^2 \sum_i (Z_i^2 + Z_i) n_i(\infty) + 4\pi e Z_0 \delta(r)\ . \tag{2-6}$$

Let the Debye length **D** be defined as follows

$$D^{-2} = 4\pi\beta e^2(\sum_i (Z_i^2 + Z_i) n_i(\infty)), \tag{2-7}$$

then the electric potential V(**r**) is readily obtained

$$V(r) = -Z_0 exp(-r/D)/r. \tag{2-8}$$

The Debye length is a measure of screening of a pure Coulomb potential Z_0/r. **D** is small at low temperature and/or the product of ion-density and its charge is large. Since most electrons are ionized in high temperature plasma, charge Z_i isusually larger than unity. Neglecting the Z_i term in Eq. (2-7) and putting $\sum_i Z_i$ to Z^*, the Debye length is written as

$$D^{-2} = 4\pi\beta e^2 Z^{*2} n_i(\infty). \tag{2-9}$$

Using the ion-coupling constant Γ and the average ion distance R_0 (=(3/4 $n_i)^{-1/3}$, **D** is expressed as

$$D = R_0/(3\Gamma)^{\frac{1}{2}} \tag{2-10}$$

If Γ value is the order of unit , the Debye length is roughly equal to the average ion distance R_0. When R_0 is larger than **D**, we can not assume ions are in Mazwell-Boltzmann distribution. This violates the assumption of Eq. 2-3. Therefore the Debye-Huckel model breaks down for Γ>1.

II-1-B Hydrogenic atom in Debye-Huckel potential.

Harris3) has calculated the energy levels of a hydrogenic atom in a Debye-Huckel potential by the variation method by using the unperturbed hydrogenic wavefunctions as a basis set. The total Hamiltonian is assumed to be the sum of the kinetic energy of a electron $\mathbf{H_0}$ and the Debye-Huckel potential $\mathbf{V(r)}$

$$H = H_0 + V(r)$$

$$H_0 = \frac{p^2}{2m}, \; V(r) = -\frac{e^2 Z}{r} exp(-r/D) \tag{2-11}$$

where the **D** is the Debye length defined by (2-9).

$$D^{-2} = 4\pi\beta \sum n_i Z_i^2 e^2$$

The eigenfunction Ψ of this atom is assumed to be written as the superposition of Hydrogenic wave function $\phi_{n,l}(r,\theta,\phi)$ with the variational coefficients $a_{n,l}$

$$\psi_{k,l} = \sum_n a^k_{n,l} \phi_{n,l}(r,\theta,\phi) \tag{2-12}$$

Since the analytical forms of the basis functions are known, the overlap and Hamiltonian matrix elements S_{ij} ($=\langle\phi_i|\phi_j\rangle$) and H_{ij} $=\langle\phi_i|H_0|\phi_j\rangle$) , respectively, can also be calculated analytically. By diagonilizing the secular matrix, coeficients a's and the energies of the orbitals can be computed. Harris uses basis functions of principal quantum number up to 9.

C. R. Smith4) applies a perturbation formalism to calculate the bound state energies in the Debye-Huckel potential. He writes the Hamiltonian of the system as the sum of unperturbed H_0 and the perturbation part $\mathbf{H'}$, i.e.

$$H = H_0 + H'$$

$$H_0 = -\nabla^2 - \frac{2}{r} + \frac{l(l+1)}{r^2}, \quad H' = -\frac{2}{r}[e^{-r/D} + 1]. \tag{2-13}$$

The perturbation energy to the first order for the (n,l) orbital is

$$\Delta E = \langle R_{n,l} | H' | R_{n,l} \rangle$$

$$= \frac{2^{2l+3}(n+1)!\,{}_2F_1(-n+l+1, -n+l+1, 2l+2, 4D^2/n^2)}{n^{2l+4}(2l+1)!(n-l+1)!(2/n+1/D)^{2n} D^{2n-2l-2}} - \frac{2}{n^2} \tag{2-14}$$

Smith presents the expression up to the second order of the perturbation energy in his paper.

His remarkable conclusion is as follows. If perturbation energy is expanded in (1/D), Eq. 2-14 will be approximated by

$$\Delta E = -2/(D+n^2). \tag{2-15}$$

From this equation, we can estimate the maximum principal quantum number of the highest bound state g^2. g^2 should satisfy the inequality

$$g^2 < D \tag{2-16}$$

The other approach for the bound states in the Debye-Huckel potential was made by F.J.Rogers et al.$^{5)}$ They choose a straight forward way of solving the wavefunctions numerically for the Debye-Huckel potential.

Though there are several differences among the results of these authors, followings are the common features for the bound states of an atom in the Debye-Huckel potential.

The energy shifts of bound states as functions of the Debye length D are shown in Figs. 2 and 3. The units of the horizontal axis are inverse proportional to the Debye length, i.e.,

$$\delta = a_0/D \tag{2-17}$$

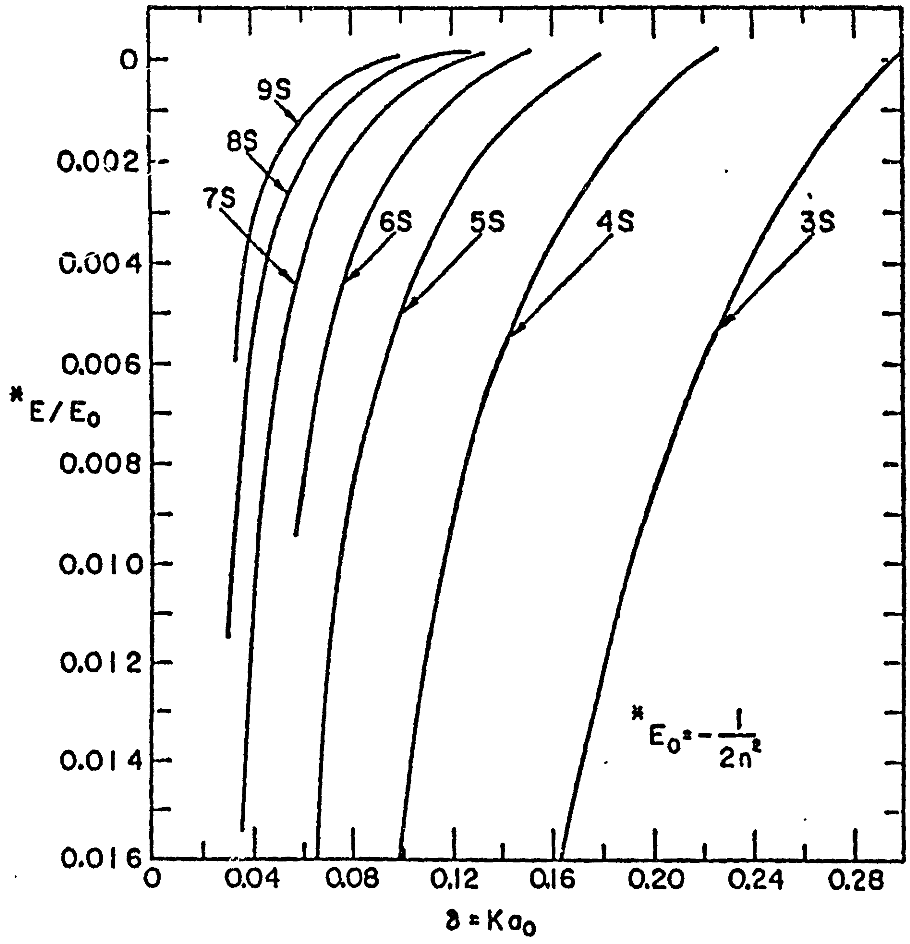

Fig. 2 Energies of s-type orbitals for a hydrogenic ion in Debye-Huckel potential. (ref. 3)

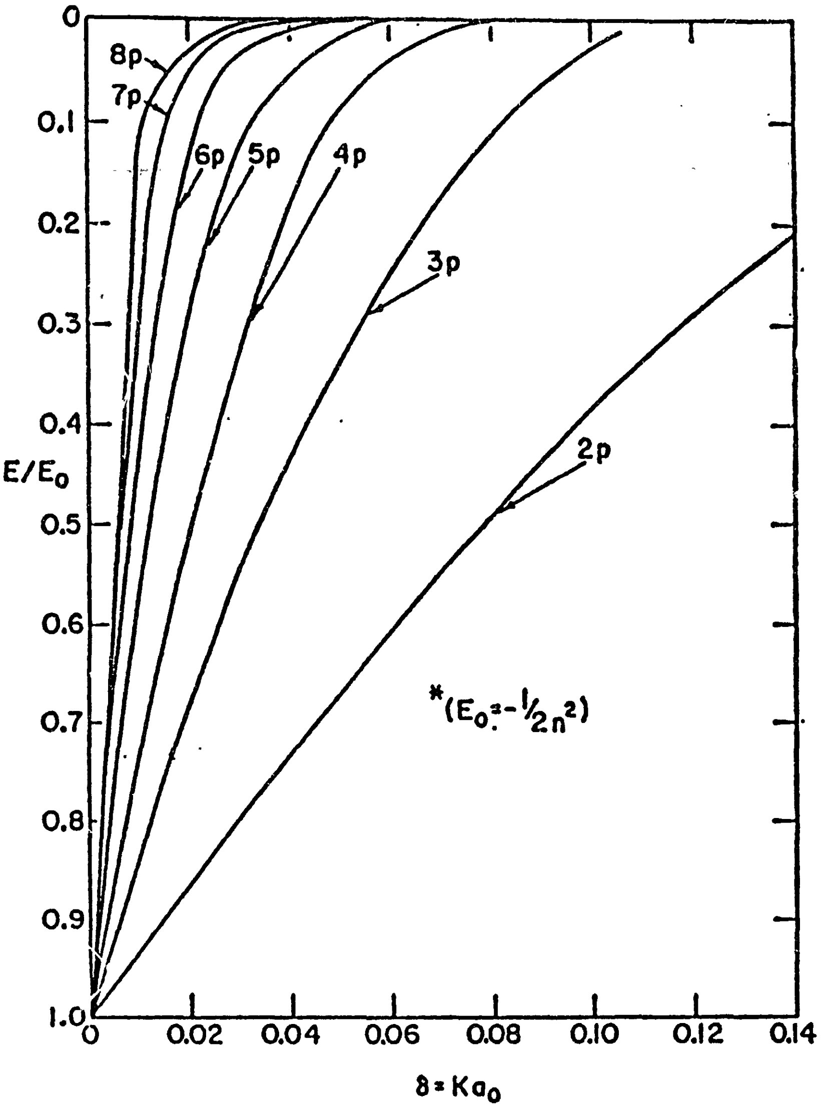

Fig. 3 Energies of p-type orbital for a hydrogenic ion in Debye-Huckel potential. (ref. 3)

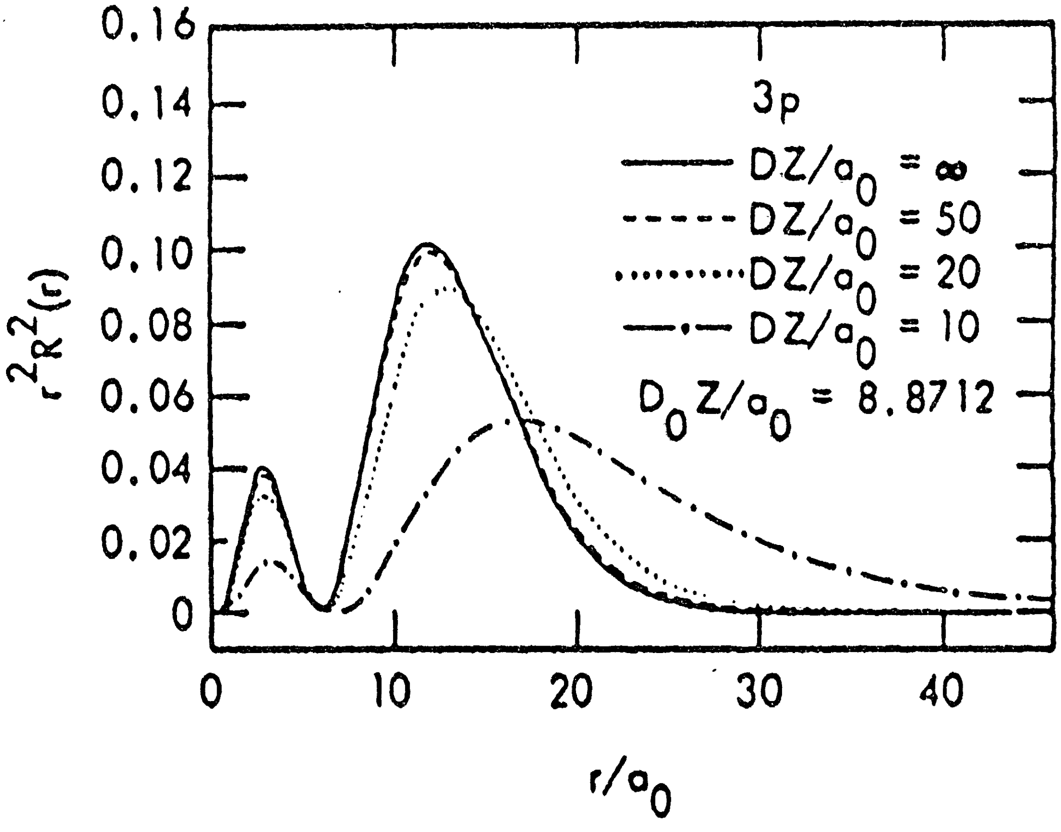

Fig. 4 Radial wave function 3p of an ion in Debye-Huckel model potential. $DZ/a_0 = \infty$ corresponds to unscreened potential. (ref. 5)

where a_0 represents the Bohr radius. The vertical axis shows the calculated energy normalized by that of an isolated hydrogenic atom, i.e., $\mathbf{E}_0 = 1/2n^2$. From Figs. 2 and 3, we can see that the states of a large principal quantum number gain their energy with the increase in the screening charge or decreasing δ. Accompanying to the energy shifts, the radial wave functions diffuse outward. The typical example is shown in Fig. 4. With the increase in the screening, the peak value decreases and the electron density flows out.

Since the energy levels are shifted upward with the decreasing **D**, the number of bound states becomes small. Figure 5 illustrates this feature. This shows that the relation between n^* and **D** is almost linear, as is suggested by Smith. The number of bound state g^* is expressed as

$$g^* = a_1 + a_2\mathbf{ZD}/a_0 \qquad (2\text{-}18)$$

the parameter a_1 and a_2 are obtained by a fitting and are summarized in table 1.

Dipole transition probability between the orbitals in Debye-Huckel potential is calculated by Roussel and O'Connell$^{6)}$ using the numerical basis function obtained by the use of the variation method. In their original paper, there are complete sets of the table of the energies obtained. The dipole transition probabilities are calculated in the length form. Figure 6 shows the the ratio of the transition probabilities of an atom in the Debye-Huckel potential to an isolated atom. When the plasma density increases (i.e., The Debye length becomes small), the transition matrix elements decrease because the energy difference between the initial and final states becomes small.

These calculations have been done for Hydrogenic ions in plasmas. It is ofcouse possible to solve the multi-electron problem in the Debye-Huckel potential. Helium likes ion in Debye-Huckel potential have been studied.$^{7)}$

II-1-C Some Problems

As mentioned above, an atom in the Debye-Huckel potential has only finite number of bound states. However, there arise a

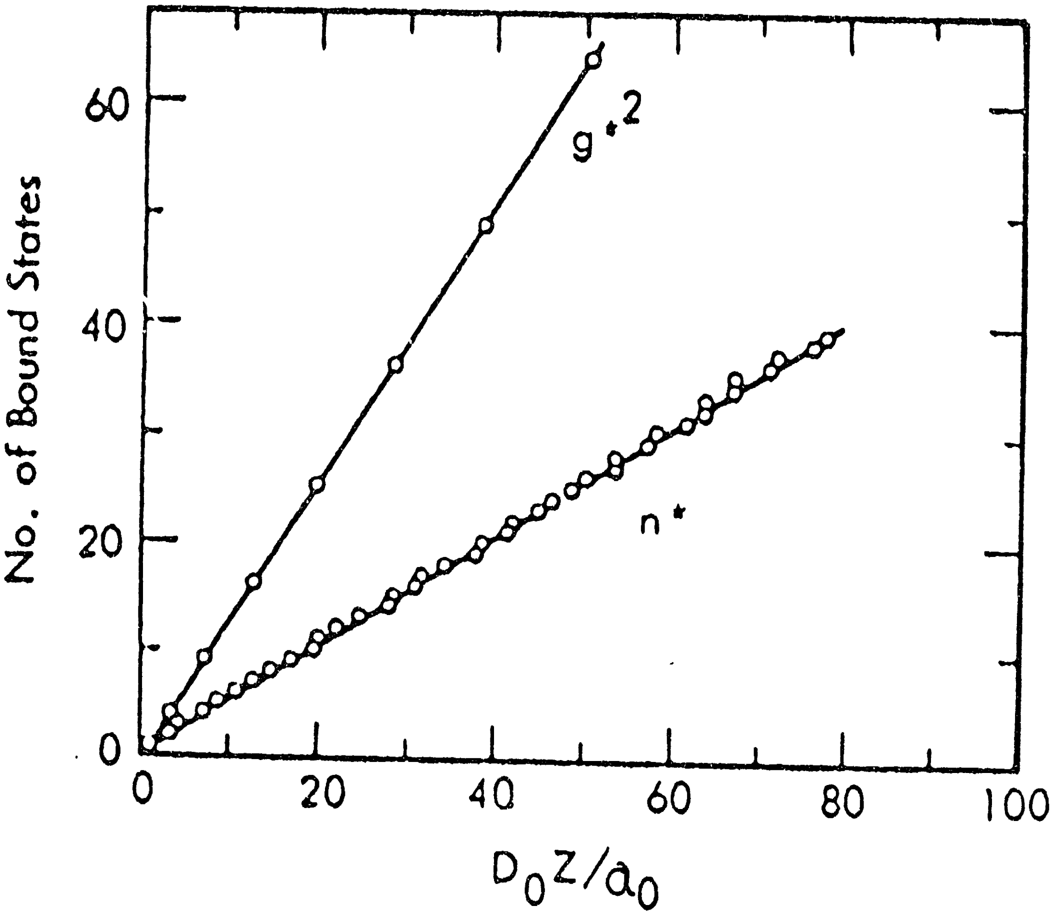

Fig. 5 Number of bound states of an ion in Debye-Huckel potential against the strength of screening. (ref. 5)

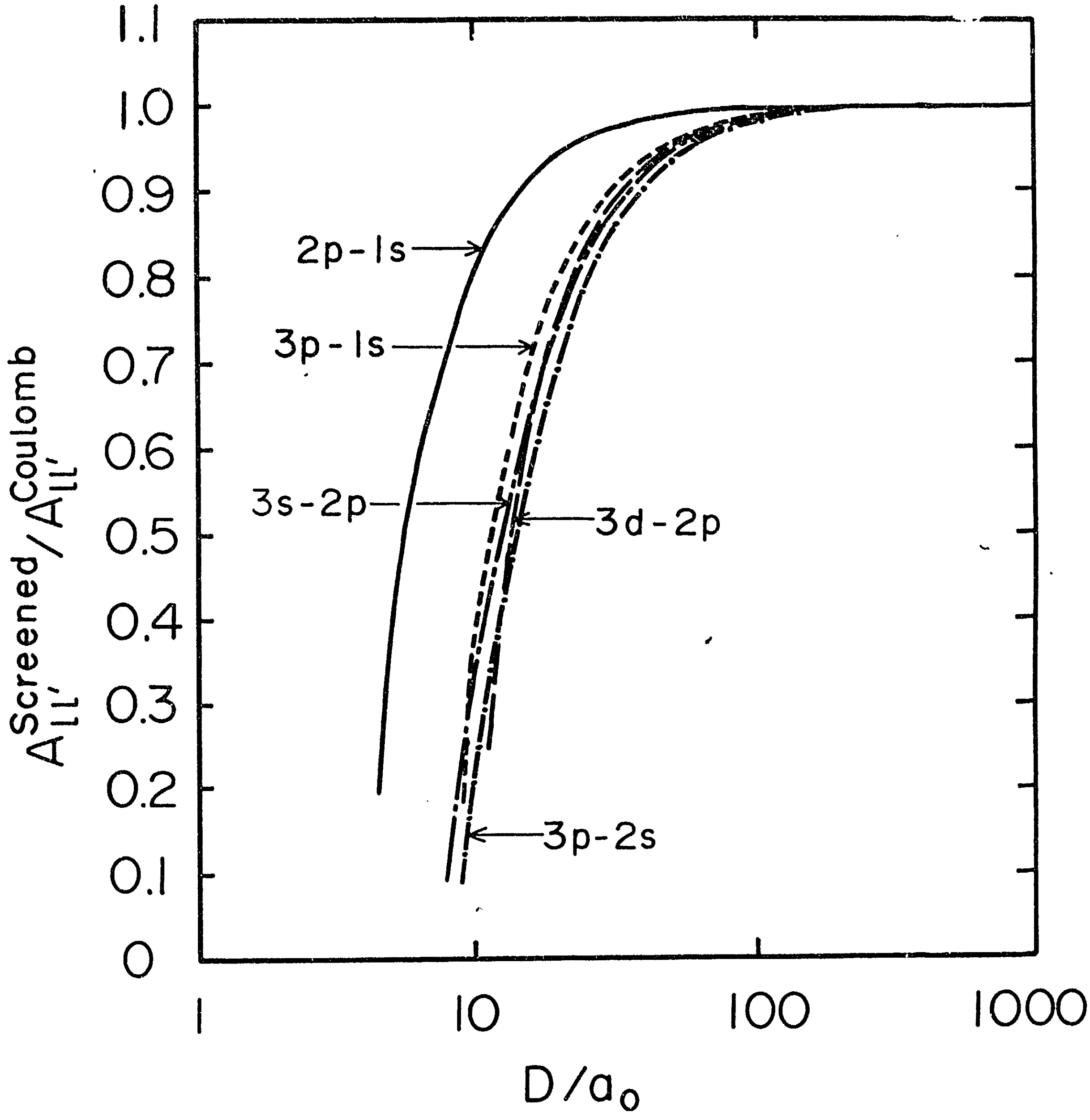

Fig. 6 Transition probabilities by the dipole approximation in Debye-Huckel potential as a function of Debye-Huckel screening length. (ref. 6)

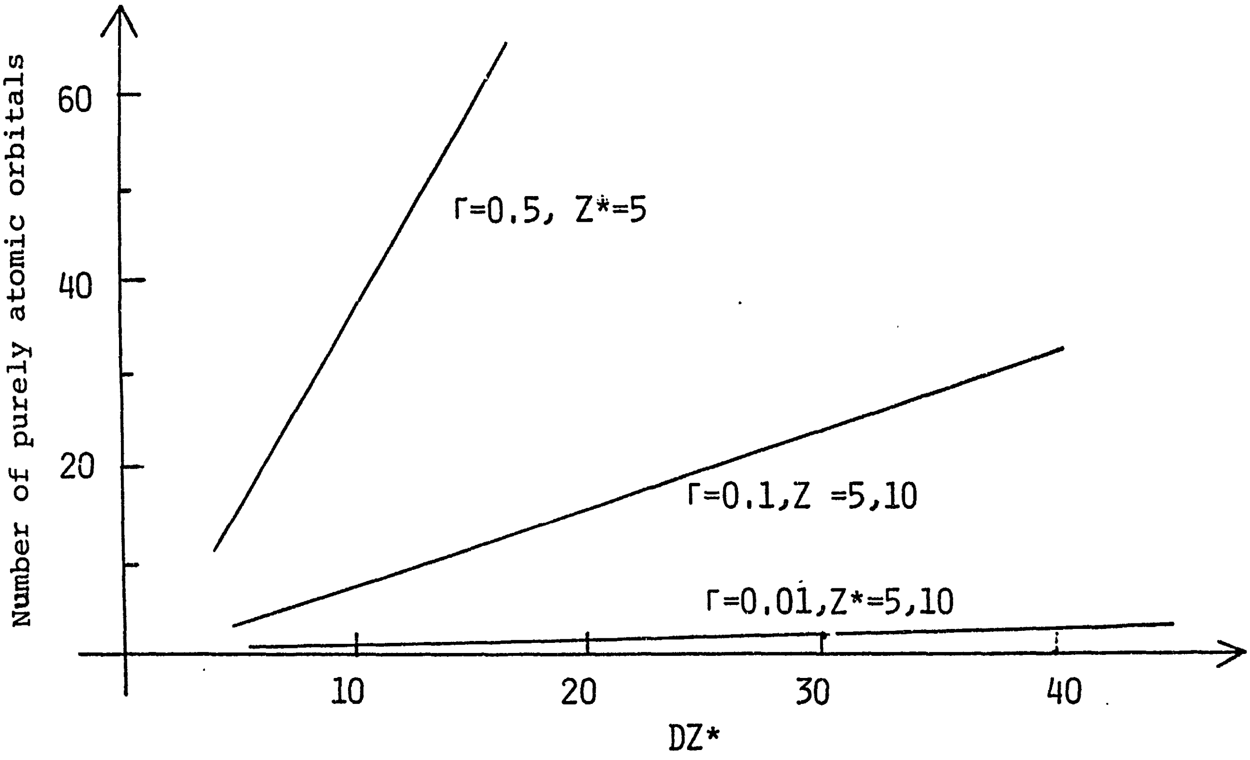

Fig. 7 Number of bound states in Debye-Huckel potential. Orbitals counted here never encounter neighboring ions.

question if all these bound states are well defined. The average radius of these bound electrons should be less than the average ion distance. If it were not the case, we must consider the mixing of the wavefunctions between ions. In a rough estimate, the average radus of n orbital $\langle r_n \rangle$ can be express as

$$Z^*/n^2 = \exp(-\langle r_n \rangle /D) / \langle r_n \rangle \tag{2-19}$$

if $\langle r_n \rangle$ exceeds the average ion distance R_0, the reality of the obtained wavefunction becomes questionable. Maximum number of n which satisfy this condition is plotted in fig. 7. This shows that some of the highly excited state, which is bound in the Debye-Huckel potential, lose their reality.

II-2 Ion-Sphere Model

II-2-A Ion-Sphere Model Potential

As mentioned in subsection II-1, the Debye-Huckel model breaks down when $\Gamma>1$. At this density and temperature region, the correlation between the ions is strong as shown in Fig. 8. The Ion-Sphere model approximates the pair correlation function in Fig. 8 with a step function. This approximation is often stated that a positive ion defines its own territory into which other positive ions can not enter. Let $\mathbf{R}_0$ be the radii of this spherical territory and call the ion-sphere radii. Since electron-electron correlation is strong too, the electron density n_e is supposed to be constant. The charge neutrality condition determines the electron density inside the ion-sphere, namely

$$n_e = 3Z/(4\pi a_0^3) \tag{2-20}$$

Here, we use the word 'Ion-Sphere' to identify the models which is based on the maximum idealization of ion-ion and electron-electron pair correlation functions. However, in some cases, the ion sphere model is referred to the treatment which is similar to the one based on the Wigner-Seitz cell: but this is not the case. The confusion over these two different ideas sometime causes troubles. Therefore we will note what ions-sphere means each time when this may happen.

The electronic potential V($\mathbf{r}$) at position $\mathbf{r}$ satisfies the Poisson eq.,

$$\frac{1}{r}\frac{d^2}{dr^2}(rV(r)) = 4\pi[en_e - eZ\delta(r)]. \tag{2-21}$$

The boundary condition for the ion-sphere model potential **V(r)** is defined from the requirments that **V**(r) is purely Coulombic in the vicinity of the origin and the electric force is zero at the surface of the ion-sphere.

$$\begin{aligned} V(r) &= -Z_0/r \qquad && for\ r = 0. \\ \frac{d}{dr}V(r) &= 0, \qquad && at\ r = R_0 \quad , \end{aligned} \tag{2-22}$$

With these conditions, The Poisson eq. (2-21) reduces to the form

$$V(r) = -\frac{eZ}{r} + \frac{eZ}{2R_0}\left[\left(\frac{r}{R_0}\right)^2 + \frac{eZ}{2R_0}\right]. \tag{2-23}$$

II-2-B Hydrogenic atom in Ion-Sphere Potential

Energy levels of hydrogenic atoms in an Ion-Sphere like potential are calculated by Skupsky[8] and Yamamoto et al[9]. Skupsky applied the perturbation method to 1s and 2p of a hydrogenic atom and pointed out the energy of the K_a X ray shifts always to the lower energy side when the ion-sphere radius becomes small, or when the ion density becomes large.

Suppose hydrogenic wavefunctions of 1s and 2p with the orbital exponents ζ1s and ζ2p are

$$\begin{aligned} \Phi_{1s} &= (\zeta_{1s}{}^3/\pi)^{1/2} exp\,(-\zeta_{1s}\, r), \\ \Phi_{2p} &= (\zeta_{2p}{}^5/\pi)^{1/2} exp\,(-\zeta_{2p}\, r)\ . \end{aligned} \tag{2-24}$$

The energy shift ΔE of the 2p - 1s optical transition in the Ion-Sphere model is

$$\Delta E = <2p\,|\,V'\,|\,2p> - <1s\,|\,V'\,|\,1s>$$

where,

$$V' = \frac{Z}{2R_0}\left(\left(\frac{r}{r_0}\right)^2 - \frac{Z}{2R_0}\right) \tag{2-25}$$

A little calculation gives

$$\Delta E = -\left[\frac{45}{2}\,\frac{1}{\zeta_{2p}^{\,2}} - 3\,\frac{1}{\zeta_{1s}^{\,2}}\right]\frac{Z-1}{2R_0}\,e^2 \tag{2-26}$$

If ζ1s = Za_0 and ζ2p = Za_0, ΔE is written as

$$\Delta E\ (\text{eV}) = 3.67 \times 10^{22}\ n_e(\text{cm}^{-3})/Z^2.$$

Skupsky extended this calculation and made it into self-consistent approximation.

Yamamoto also uses the perturbation approximation and calculated the energy shifts. The interaction Hamiltonian of a hydrogenic ion in Ion-Sphere of radius R_0 is

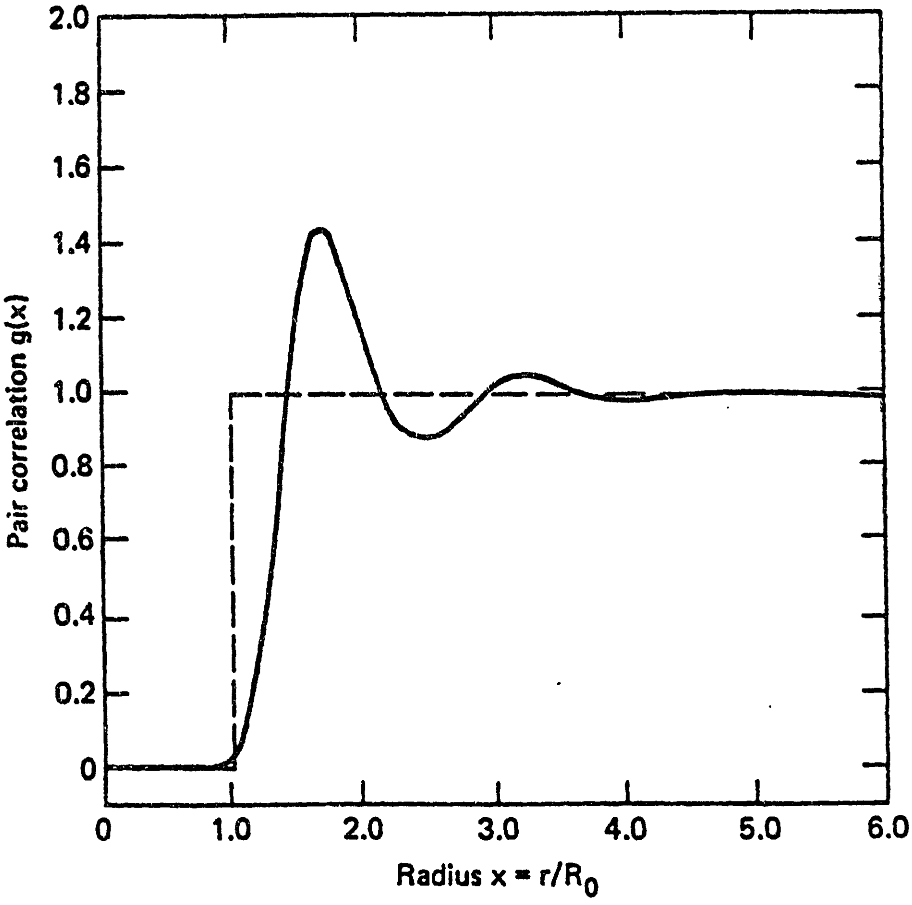

Fig. 8 The pair correlation function. The broken line shows the results by the Ion-Sphere model.

$$V = e^2 \int_0^\infty \frac{n_e(r')}{|r-r'|} dr' , \quad n_e(r) = \begin{cases} 3(Z-1)/(4\pi R_0) & \text{for } r < R_0 \\ 0 & r > R_0 \end{cases} \tag{2-27}$$

The perturbed energy $E_{n,l}$ for the hydrogenic wave functions of principal and azimuthal quantum numbers, n and l respectively, are

$$\begin{aligned} \Delta E_{n,l} &= \langle n,l \mid V' \mid n,l \rangle \\ &= \frac{(Z-1)e^2}{2a_0} \frac{a_0}{R_0} [3 - (\frac{a_0}{R_0})^2 \frac{n^2}{2Z^2} (5n^2 + 1 - 3l(l+1))] \\ &+ (Z-1)e^2 \int_{R_0/a_n}^{\infty} [u - \frac{3}{2} \frac{a_n}{R_0} u^2 + \frac{1}{2} (\frac{a_n}{R_0})^3 u^4] a_n^{\,2} R_{nl}^{\,2} \, du \end{aligned} \tag{2-28}$$

where

$$u = r/a_n, \qquad a_n = na_0/2Z$$

Figure 9 plots the energy shift of several levels against the plasma density. When the plasma density increases every orbital energy goes up and high n wave functions vanish into the continuum. This phenomenum corresponds to the continuum lowering in this quantal case. However, the reality of these highly excited orbitals, which have the amplitude outside the sphere and thus vulnerable to the perturbers, is questionable.

Yamamoto et al added non-spherical perturbation Hamiltonian to this model. This additional potential causes a Stark shift to the energy of the orbitals. Concerning to this effect, see subsection IV-1.

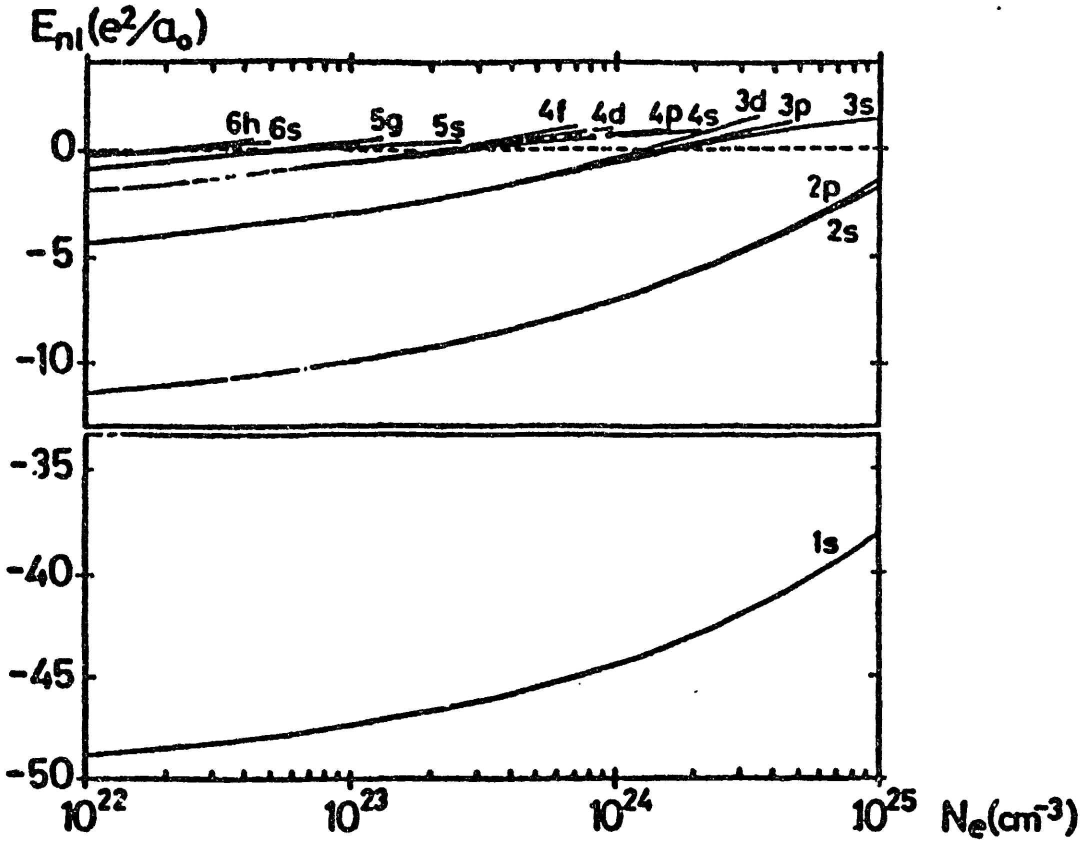

Fig. 9 Density-dependence of the energy-level of a hydrogen-like neon calculated by the ion-sphere model with a Hartree potential: $E_{nl} = -Z^2/2n^2 + \Delta E_{nl}$. (ref. 9)

II-3 Stewart-Pyatt Model

Since the Debye-Huckel model in subsection II-1 is valid only for high temperature and thin plasma, the velocity distribution of electrons can be the Maxwellian. In order to extend this model to high plasma, the Fermi-Dirac distribution should be used without relying on the high temperature expansion.

Let's write the Poisson Eq.(2-1) again.

$$\nabla^2 V(r) = -4\pi e^2\left(\sum_i z_i n_i(r) - n_e + z_0\delta(r)\right) . \tag{2-1}$$

In the present model electrons are in the Fermi-Dirac Distribution.

$$n_e(r) = a\, n_e(\infty) \int_{eV(r)}^{\infty} \frac{\varepsilon^{-1/2}}{1+exp[\beta(\varepsilon-eV(r)+\mu)]}\, d\varepsilon \tag{2-29}$$

The integration of RHS of eq. (2-29) starts from the energy at which the kinetic energy of electron is positive.

Positive ions is in the Maxwell distribution as are same as the Debye-Huckel model.

$$n_i(r) = n_i(\infty) exp[-\beta z_i V(r)] \tag{2-30}$$

Now we introduce new non-dimensional variables x=**r**/**D** with the Debye-length defined in (2-7) and potential y $= \beta$ e**V**. Equation (2-1) is written as[4]

$$\frac{1}{X}\frac{d^2}{dX^2}(XY) = \frac{1}{Z^2+1}\left[\frac{F(Y-a,Y)}{F(-a)} - \frac{<Z\, exp(-Z^* Y)>}{<Z>} + c(X)\right] , \tag{2-31}$$

where <> means the averaging with respect to ions weighted $n_i(\infty)$ and Z^* stands for $<Z^2>/<Z>$. The Fermi integral $F(\eta,Y)$ is defined as

$$F(\eta,Y) = \int_Y^{\infty} \frac{t^{1/2}\,dt}{1+exp(t-\eta)} \tag{2-32}$$

a in eq (2-29) is the normalize constant as defined from

$$n_e(\infty) = \frac{2(2\pi m_e k_B T)^{3/2}}{h^3} \frac{2}{\sqrt{\pi}} F(-a,0) \; . \tag{2-33}$$

The final form of the Poisson equation is read as

$$\frac{1}{X}\frac{d^2}{dX^2}(XY) = \frac{1}{1+Z^*}[\frac{F(Y-a,Y)}{F(-a)} - exp(-Z^*) + c(X)] \, . \tag{2-34}$$

This equation and the resultant potential are usually called as Stewart-Pyatt equation and potential, respectively. The first term of RHS in eq. (2-34) is brought from electrons and the second is from positive ions and the third is from the central nuclear charge.

Let's consider the solution of Eq. 2-34 in two extreme cases.

1) When $z^*Y<<1$, the potential **V(r)** or Y is decided mainly by the spatial distribution of the positive ions. Eq (2-34) reduces to the Debye-Huckel equation

$$\frac{1}{X}\frac{d^2}{dX^2}(XY) = \frac{1}{1+Z^*} + C(X) \tag{2-35}$$

2) When $Z^*Y>>1$ (i.e., $Y>>1/Z^*$), the dominant features of the potential are determined not by the positive ions but the electrons. If the average charge of positive the ions Z^* is much larger than unity, $F(y-a)/F(-a)$ is nearly equal to unity for $1/Z^*<Y<1$. In this case the solution of Eq. (2-34) is identical to that for the ion-sphere potential,

$$\frac{1}{X}\frac{d^2}{dX^2}(XY) = Y + C(X) \tag{2-36}$$

In general, condition 1 is satisfied for large **x** (= **r/D**). On the contrary, in the limit of X = 0, condition 2 holds. Therefore, the Stewart-Pyatt equation gives the Debye-Huckel potential at infinity and the ion-sphere potential at the origin.

Now we remind that there are bound and free electrons, which were not treated separately in the previous discussion. Let $n_f{}^e(r)$ and $n_b{}^e(r)$ be the number densities of the free and bound electrons, respectively. The potential $V_f(r)$ felt by a free electron satisfies the same Poisson Eq. (2-1)

$$\nabla^2 V^f(r) = -4\pi e[\sum_i z_i n_i(r) - n_e^f(r) - n_e^b + z_0\delta(r)] \qquad (2\text{-}37)$$

If the density of bound electron is known, its contribution to $V^f(r)$ can be represented by modifying the central 'lear charge Z_0. Using a new effctive ncharge K_0 thus obtained, the Poisson Eq.(2-37) is in the form

$$\nabla^2 V^f(r) = -4\pi e[\sum_i z_i n_i(r) - n_e^f(r) + K_0\delta(r)] \qquad (2\text{-}38)$$

Free electrons obey the Fermi-Dirac distribution and we write

$$n_e^f = a\, n_e(\infty)\int_0^\infty \frac{\varepsilon^{-1/2}}{1+\exp[\beta(\varepsilon - eV(r)+\mu)]}\,d\varepsilon\,, \qquad (2\text{-}39)$$

$$n_e^f(\infty) = n_e(\infty)$$

The boundary condition (2-39) means that there is no bound electron at infinity.

Now we define a non-dimensional potential for free electrons V(x) by $V_f(r)$. Eq. (2-38) is written as

$$\frac{1}{X}\frac{d^2}{dX^2}(XY) = \frac{1}{1+Z^*}[\frac{F(Y-a,0)}{F(-a)} - \exp(-Z^*) + K_0\delta(X)] \qquad (2\text{-}40)$$

The LHS of Eq. (2-40) is a function of the free electron potential and the RHS is of the that of total electron. From Eq. (2-39) the boundary condition for V is

$$V(\infty) = V^f(\infty) \qquad (2\text{-}41)$$

Let **S**(x) be the RHS of Eq. (2-40) with the known Y in Eq. (2-34):

$$\frac{1}{X}\frac{d^2}{dX^2}(XY) = S(X)\,,$$

$$S(X) = \frac{1}{1+Z^*}[\frac{F(Y-a,0)}{F(-a,0)} - \exp[-Z^* Y] + K_0\delta(X)] \qquad (2\text{-}42)$$

A formal integration of the Poisson Eq. (2-42) is written as

$$V(X) = \int_0^X S(t)\,dt - \frac{1}{X}\int_0^X S(t)t^2\,dt + J \qquad (2\text{-}43)$$

A parameter J which determines the behaviour of the potential at the origin is decided by the boundary condition (2-41) as

$$J = -\int_0^{\infty} S(t)t dt = V(0) \tag{2-44}$$

Though numerical integration leads the solution v(x), we can obtain an approximate solution in the following way.

Suppose y(x) and v(x) are connected smoothly at x_1. The position of x_1 is decided later. For $x > x_1$, y is given by the Debye-Huckel potential

$$Y = \frac{C}{X} e^{-X} \tag{2-45}$$

For $x < x_1$, y is the ion-sphere potential.

$$Y = \frac{K}{X} - J + \frac{X^2}{6(Z^*+1)} \tag{2-46}$$

The conditions that both solutions are continuous and smooth at x_1 yield

$$J = \frac{X_1}{Z^*+1}(1+\frac{X_1}{2})$$

(2-47)

$$K = \frac{X_i}{Z^*+1}(1+X_1+\frac{X_i^2}{3})$$

The connecting poinm x_1 is obtained by the neutrality condition

$$4\pi\int X^2 Y dX = Z^* . \tag{2-48}$$

II-4 Continuum Lowering in the Three Models

With an increase in the plasma density, energies of the bound states shift upward. This shift is described in the models introduced in this section. This effect is observed experimentally in the X-ray emission spectrum as the edge shift of continuous X-ray. This phenomenum is often called as "continuum lowering" and used as a method of determining the plasma density and temperature. Any model for an ion in screened potentials can give an explanation of this continuum lowering but the estimation of its magnitude is different each other.

By the Debye-Huckel model, the continuum lowering C_l is calculated by subtracting the pure Coulomb potential Z_0/r from $V(r)$ in Eq. (2-8).

$$C^l = \lim_{r\to 0} \left[\frac{Z_0 exp(-r/D)}{r} - \frac{z_0}{r}\right] \tag{2-49}$$

In the ion-sphere model, $C_l v$ is given by the additional term $-eZ/2Z_0$ in Eq. (2-23). For the Stewart-Pyatt Model, C_l is given by J in (2-44). (See Table 2)

TABLE 2 Continuum Lowerings by Classical Models

Models	Estimation of continuum lowering
Debye-Huckel	$-Z_0/D$
Ion-Sphere	$-eZ/2R_0$
Stewart-Pyatt	$-J$

III Semi-Classical Treatments (Thomas-Fermi Model and its extensions)

For atoms in strongly coupled plasmas, i.e., $\Gamma >> 1$, Thomas-Fermi model is frequently used because of the following reasons. First, this model does not assume uniform electron distribution, while the ion-sphere model dose. Second, equation of state and thermodynamic variables can be easily obtained in this model. Many workers have extended and modified the original Thomas-Fermi model which is for the zero temperature. Cowan and Ashkin[11] derived the equation with the exchange interaction included and valid for at finite temperature. Von Weisacker[12] and Plaskett[13] introduced so called weisacker or gradient correction. Thomas-Fermi model with this corection is often called **Quantum Statistical Model.** From the viwpoint of the density functional method, this correction can be treated systematically. Taking the electron density as a fundamental variable, Honenberg, Kohn and Sham[14,15,16] introduced the basic idea of the density functional method. Marmin[17] and Pellow[18] extended this model to the finite temperature case.

The ion-sphere model is based on the most simplest model of the ion-ion and the electron-electron correlations. But the original Thomas-Fermi model dose not take these into account. The Thomas-Fermi model can describe features of atoms in plasma only if these correlation is stated in the form of boundary condition. If not, the Thomas-Fermi model can handle only an isolated atom or ion. When the ion-sphere type boundary condition is introduced, the Thomas-Fermi model is called **confined Atom Thomas-Fermi Model (CATFD).** The boundary condition of Debye-Huckel type is also applied to the Thomas-Fermi model. This version is called the **Debye-Huckel Thomas-Fermi Model** (**DHTF** for short).

Results of Thomas-Fermi model may depend on two points, one is the accuracy of density functional approach and the other one is the bpindary condition of TF-model which must reflect the real enviroument of atoms in plasmas. We briefly introduce the Thomas-Fermi model from the standpoint of the density functional method. The review article by N.H.March[18] is usuful for the detailed discussion on the Thomas-Fermi model and that by Gupta and Rajagopal[19] for the density functional method.

III-1 Basic Formalism

The total Hamiltonian **H** for an interacting electron gas at finite temperature in an external potential **V**(r) is written as the sum of the kinetic **T**, potential energies and the interaction energies between electrons **U**, i.e.,

$$\mathbf{H} = \mathbf{T} + \mathbf{V} + \mathbf{U}. \tag{3-1}$$

With electron wavefunction $(r_1, r_2,,,, r_N)$, each term in RHS of eq 3-1 is written

$$T = \frac{\hbar^2}{2m} \int_i \nabla\psi^*(r)\nabla\psi(r) \quad dr^N ,$$

$$V = \int \psi(r)^* V\psi(r)\,dr^N , \tag{3-2}$$

$$U = \frac{1}{2} \int \psi(r)^* u(x_i - x_j)\psi(r)\,dr^N ,$$

where $u(x_i-x_j)$ stands for the interaction energy between electrons.

The partion function **Z** is given by

$$Z = \sum_K exp[-\frac{E_K - \mu N}{k_B T}] \tag{3-3}$$

Here E_k is the energy eigenvalues of ω_k and μ represents the chemical potential. N is the total number of electrons in the system. Since the grand canonical distribution ω_K is given as

$$w_K(E_K) = exp[-\frac{E_K - \mu N}{k_B T}]/Z, \tag{3-4}$$

the density matrix is

$$\rho(x, x') = w_K \Psi_K(x)\Psi_K{}^*(x')$$

$$(3\text{-}5)$$

$$= \sum_K exp[\frac{-E_K - \mu N}{k_B T}]\psi_K(x)\psi_K{}^*(x')$$

Therefore the electron density n(r) can be written

$$n(r) = Tr[\rho_0 \psi^*(r')\psi(r)]|_{r'=r} \tag{3-6}$$

Now the grand potential Ω of the system becomes

$$\Omega = Tr[\rho(H-\mu N+\frac{1}{\beta}ln\rho)] \tag{3-7}$$

If the system is in thermal equilibrium, the grand potential Ω takes the minimum. The density functional method is based on the idea that the density matrix ρ is the unique functional of the electron density n(r). Correct n(r) minimizes the grand potential . Since the density matrix is the unique functional of n(r), the energy expectation value <H> is also the functional of n(r).

We define F(n)

$$<H> = Tr[\rho H] = \int V(r)n(r)dr + F[n(r)] \tag{3-8}$$

Honenberg and Kohn$^{15)}$ define G[n(r)] by F[n(r)] as

$$F[n(r)] = \frac{1}{2}\int \frac{n(r)n(r')}{r-r'}drdr' + G[n(r)] \tag{3-9}$$

Here G[n(r)] represents the kinetic energy of electrons and exchange and correlation interactions betweeen electrons. Therefore G[n(r)] can be written as

$$G[n(r)] = \frac{1}{2}\int \nabla r \nabla r' n(r,r')|_{r=r'} dr + \frac{1}{2}\int \frac{c_2(r,r')}{|r-r'|}drdr' \tag{3-10}$$

Now we define $g_r[n]$ by

$$G[n(r)] = \int g_r[n]\,dr \tag{3-11}$$

though G[n(r)] is a unique functional of n[r], $g_r[n]$ is not unique. Indeed, $g_r[n]$ with an arbitrary functional h_r of n[r]

$$g_r[n] = g_r[n] + \sum_{i=1}^{3} \frac{\partial}{\partial x_i} h_r V[n] \tag{3-12}$$

gives the equivalent results.

Suppose $g_r[n]$ is expanded as

$$g_r[n] = g_0(n(r)) + \sum_{i=1}^{3} g_i(n(r))\nabla_i n(r)$$

$$+ \sum_{i,j} g_{i,j}^{(1,1)}(n(r))\nabla_i n(r)\nabla_j n(r) \tag{3-13}$$

$$+ g_{i,j}^{(2)}(n(r))\nabla_i \nabla_j n(r) + \ldots$$

From the facts that $g_r[r]$ is invariant under a rotation of r and that addition of an arbitrary divergence $h_r[n]$ g_r is known to have the form

$$g_r[n] = g_0 + g_2^{(2)}(n)(\nabla n)(\nabla n) +$$

$$+ [g_4^{(2)}(n)(\nabla^2 n)(\nabla^2 n) + g_4^{(3)}(n)(\nabla^2 n)(\nabla n \nabla n) \tag{3-14}$$

$$+ g_4^{(4)}(n)(\nabla n \nabla n)^2] + \ldots$$

g_0, g_2 and g_4 are not functionals but the functions of n(r). The second term in eq 3-14 introduces the gradient correction.

III-1-a **Thomas-Fermi Equation**

Now we derive the usual Thomas-Fermi equation. For this purpose we neglect the gradient term of the functional of T and the exchange and correlation terms in eq 3-10. Furthermore, we approximate the g_r by its form of a free electron gas at zero temperature. i.e.,

$$g_r[n] = \frac{3}{10}[K_f(n)]^2 n \qquad (3\text{-}15)$$

where K_f is Fermi momentum given by

$$K_f = (3\pi^2 n)^{1/3} \qquad (3\text{-}16)$$

The total energy of this system can be written as

$$E_v = \int v(r)n(r)\,dr + \frac{1}{2}\int \frac{n(r)n(r')}{r-r'}\,drdr' + \frac{3(3\pi^2)^{2/3}}{10}\int n(r)^{5/3}dr \qquad (3\text{-}17)$$

Since temperature T is zero, the condition of minimizing E determines the electron density n(r), namely,

$$\delta[E_v(n) - \mu\int n(r)dr] = 0\,. \qquad (3\text{-}18)$$

Equation 3-18 yeilds

$$V(r) + \int \frac{n(r')}{r-r'}\,dr' + \frac{1}{2}\int (3\pi^2)^{2/3}[n(r)]^{2/3} - \mu = 0 \qquad (3\text{-}19)$$

If we define the internal potential $v^i(r)$ as

$$v_i(r) = \int \frac{n(r')}{|r-r'|}\,dr'\,. \qquad (3\text{-}20)$$

then simultaneous eqs.

$$\nabla^2 v_i(r) = -4\pi n(r)$$
$$n(r) = (1/3\pi^2)[2(\mu - ev(r) - ev_i(r))]^{3/2}, \qquad (3\text{-}21)$$

are equivalent with eq. 3-19. Elminating n(r) from eqn. 3-21, we can obtain the well known Thomas-Fermi eq., that is,

$$\nabla^2 v_i(r) = -\frac{2^{7/2}}{3\pi}[\mu - ev(r) - ev_i(r)]^{3/2} . \qquad (3\text{-}22)$$

In the Thomas-Fermi Model in the case of a finite temperature, n(r) is replaced by

$$n(r) = \frac{1}{(2\pi)^3}\int \frac{1}{1 + exp(\beta[p^2/2m + ev(r) + ev_i(r) - \mu])}\,dp$$

(3-23)

Here we have used the fact that the total wavefuction should be anti-symmetrized because an electron is a fermion.

III-1-b Exchage interaction and Gradient correction

Approximating $g^r[n]$ in eq. 3-14 by eq. 3-1, we obtain Thomas-Fermi equation with the exchange interaction. An accurate calculation 11) shows g^0 in eq 3-14 is in the form

$$g_0 = \frac{3}{10}(3\pi^2 n)^{2/3} + e_{ec}(n) \qquad (3\text{-}24)$$

where e^{ec} represents the exchange and correlation interactions. When the electron corelation is neglected, e_{ex} is expressed as

$$e_{ex}(n) = -(1/\pi)[3\pi^2 n(r)] \qquad (3\text{-}25)$$

The second term in eq 3-11 is known to be the gradient correlatin. Comparing polalizability of the electron gas calculated by the use of of Random phase approximation 17) , Perror shows $g^2(n)$ is written as

$$g^2(n) = -\frac{2^{1/2}}{24}\pi^2\beta^{3/2}\frac{d}{d\eta}\left(\frac{1}{I_{1/2}(\eta)}\right), \qquad (3\text{-}26)$$

where I_n is the standard Fermi integral defined by

$$I_n(\eta) = \int y^n \frac{dy}{1+e^{y-\eta}} , \tag{3-27}$$

III-2 Thomas-Fermi Model with an Ion-Sphere Boundary

In this subsection we solve the Thomas-Fermi equation Eq. 3-21 or 3-22 with an ion-sphere boundary condition. Since Eq 3-21 is a simultaneous eqs., two boundary conditions are needed for each n(r) and V(r).

An ion-sphere radius R_0 is calculated using the ion density n_i as

$$n_i = (4\pi R_0^3/3)^{-1} \tag{3-28}$$

Electrons are distributed inside the sphere R_0. Therefore charge neutrality condition is written

$$\int n(r)dr = z \tag{3-29}$$

This condition actually determines the chemical potential μ.

At the surface of the ion-sphere the electric force should be zero: that is

$$dV/dr|_{R_0} = 0 \tag{3-30-a}$$

The potential is same as that of bare ion at the origin.

$$V(r) = -eZ/r, \qquad for \quad r = 0. \tag{3-30-b}$$

Finally, electron density must be connected smoothly with that of the neighbouring ion-sphere. This condition is written as

$$dn/dr|_{R_0} = 0 \tag{3-31}$$

Without the Weisacker correlation, the electron density diverges at the origin because the potential is supposed to be r^{-1}.
With the Weiszacker correlation, the boundary condition Eq. (3-30-b) can be replaced by the electron density at the origin. These four boundary conditions charcterizes the ion-sphere Thomas-Fermi model. Typical results by this model will appear in the sub-section 3-.

III-3 Thomas-Fermi Model with a Debye-Huckel Boundary

An ion-ion interaction has been competely simplified in the ion-sphere-like Thomas-Fermi model in subsection III-2. Cowan and Kirkwood20 investigated a Thomas-Fermi model with the boundary condition of the Debye-Huckel type. Let $Q^+(r)$ be the sum of charge densities of electrons and ions around a positive ion. $Q^+(r)$ is written as

$$Q^+(r) = Zn^{i+}(r) - en^{+e}(r)\,, \tag{3-32}$$

where n^{+i} and n^{+e} stand for number densities of ions and electrons around the positive ions, respectively.

The Poisson Eq. 3-32 for potential $V^+(r)$ felt by an electron is

$$\begin{aligned} \nabla^2 V^+(r) &= -4\pi Q^+(r) \\ &= -4\pi e(Zn^{i+}(r) - n^{+e}(r)) \end{aligned} \tag{3-33}$$

$V^+(r)$ is Coulombic at the origin and zero at infinity, i.e.

$$\begin{aligned} V^+(r) &= -Ze/r \qquad && at\ r = 0 \\ V^+(r) &= 0 && at\ r = \infty \end{aligned} \tag{3-34}$$

Now we assume that the thermal distribution of electrons is the Fermi-Dirac distribution and that of ions is the Maxwellian. That is

$$\begin{aligned} n^{+i} &= n^i(\infty)exp[-\beta zeV^+(r)] \\ n^{+e}(r,p) &= n^e(\infty)\,p_2/[1+exp(\beta(p^2/2m + eV^+ - \mu))]\,. \end{aligned} \tag{3-35}$$

Integrating Eq. (3-35) with respect to the momentum p, we obtain

$$n^{+e}(r) = \frac{8\pi e^2}{h^3}\int \frac{p^2dp}{1+exp[\beta(p2/2m + eV^+(r) - \mu)]} \tag{3-36}$$

Here we utilize the fact that each state of an electron occupies a volume h_3 in the phase space.

The potential $V^+(r)$ and n^{i+} can be obtained by solving Eqs. (3-35), and (3-36) with the boundary condition (3-34).The formalism mentioned above may be regarded as an extention of the Stewart-Pyatt model (see section II-3) using the idea of Thomas-Fermi model.

The contribution of positive ions to various physical quantities is large for large β, that is for low temperature plasma. In fig . 10, pv/kT (p and v are pressure and volume of the system, respectively, in this context.) is plotted against T which is calculated by the ordinary Thomas-Fermi model for an isolated atom and the present Debye-Huckel Thomas-Fermi model. These show that the results by both of the models agree each other at the high temperature limit , i.e when T is higher than 100 eV.

The formalism described above does not distinguish the bound electrons from the free ones. Zakowicz et al [21)] proposed an alternative method by which they calculated the effective charge of the ions Z^{eff} in a straightforward manner. They also pointed out the fact·that the number of bound electrons calculated by the Debye-Huckel-Thomas-Fermi model shows a strange behaviour. Following their discussion, we call the electrons bound whose energies are less than the binding energy. Electric potential now must satisfies the equations below. (See ref. 21 for the detailed derivation of the equations).

$$\nabla^2 V^+ = 4\pi e[8\pi \int_0^\infty \frac{p^2 dp}{(2\pi\hbar)^3} \frac{1}{1+\exp(\beta(\frac{p^2}{2m}+\eta))} - Z_{eff} n_0 e^{-Z_{eff} eV^+(r)}$$

$$\frac{8\pi}{(2\pi\hbar)^3} \int_0^\infty \frac{p^2 dp}{1+\exp(\beta(\frac{p^2}{2m}-\eta))} = Z_{eff} n_i(\infty)$$

$$Z_{eff} = (4\pi)^2 \int_0^\infty drr^2 \int_{\sqrt{2m_e V^+(r)}}^\infty \frac{2p^2 dp}{(2\pi\hbar)^3 \left\{1+\exp(\beta(\frac{p^2}{2m}+\eta))\right\}}$$

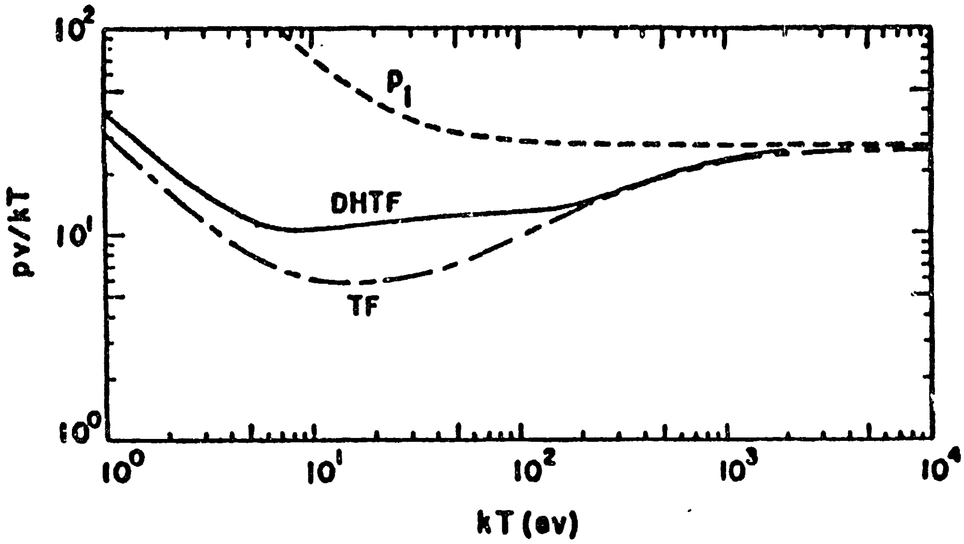

Fig. 10 pv/kt against temperature for iron at normal solid density. Results of Debye-Huckel and ion-sphere models are compared. (ref. 20)

Fig.$_{11a}$ shows the fractions of the bound electrons as a functions of temperature. The number of the bound electrons increases with the increase in temperature at low temperatures if compared with the result of Ion-sphere-Thomas-Fermi Model shown in Fig.11b The value in question is about 1.25 for $T=10^5$ and $n=10^{23}$ cm^{-3}. As mentioned in section II-1, the Debye-Huckel model breaks down at Γ equals unity. So it may leads to an error if we use the Debye-Huckel Model at this region. However, this strange behaviour occures for the following reasons. At high temperatures ions have a large kinetic energy and can penetrate into the territories of other ions. This contradicts to the assumption in Ion-Sphere model which prohibit this penetration. The pulling of electrons by the strong attractive Coulomb potential will surpass their removal by thermal ionization. Zakowicz showed an appreciable fraction of bound electrons appears at the distance larger than the mean distance between ions. So the overestimate of bound electron stems from the fact that the electron which are loosely bound and easily affected by the perturbation from any external fields(i.e., the electrons in quasi-stational state) is regarded to be bounded. In order to get a corrct fruction of bound electrons in the Debye-Huckel model, the definition of the bound electron should be modified. The similar discusion is made by Carson and Hollingsworth 22).

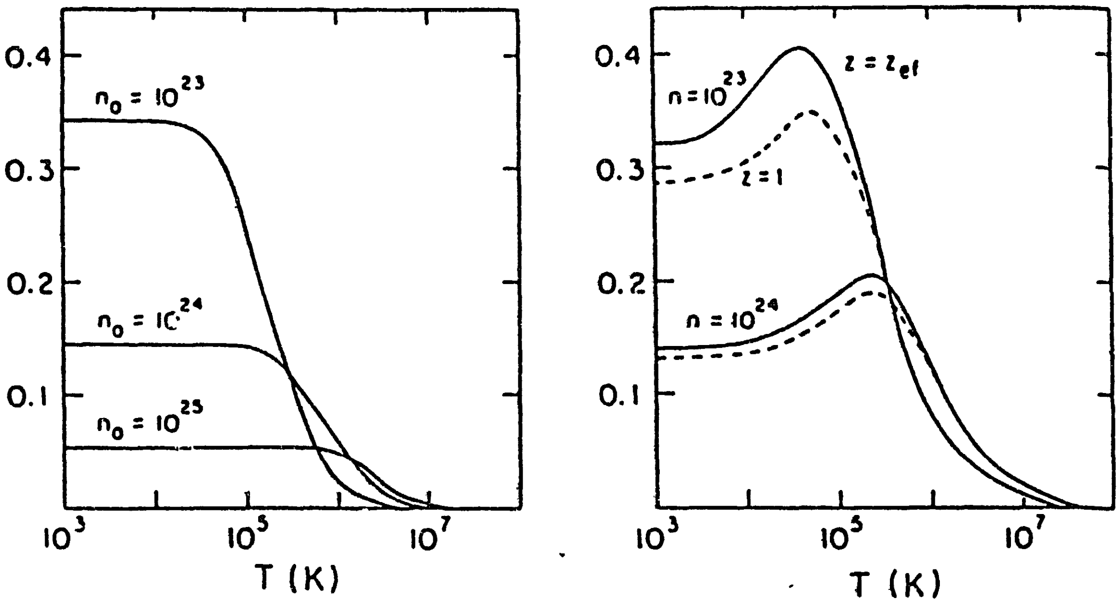

Fig. 11 Fraction of bound electrons calculated by Ion-Sphere Thomas-Fermi model (a) and Debye-Huckel Thomas-Fermi model (b). (ref. 21)

III-4 Thomas-Fermi Model for Multi-Component Plasma

The Ion-sphere radius can be calculated from the plasma density in the case of the ion-sphere Thomas-Fermi model of one component plasma as discussed in subsection III-2. For multi-component plasma, ion-sphere radius for each component are not known. They are determined by the condition that the fermi-level for each ion is the same, in other word the chemical potential are common to all the ion spieces. The Debye-Huckel Thomas-Fermi model can also be extended for a multi-component plasmas. See ref. 23 and 24 for the detail.

III-5 Thomas-Fermi Shell Model

Various Thomas-Fermi Models in the previous sections do not distinguish the bound electrons from the free ones. The number of electrons that are inside the sphere R^0 is given as

$$\frac{1}{h^3}\int 4\pi r^2 dr \int \frac{8\pi p^2 dp}{1+exp[\beta(p^2/2m-eV+\mu)]} \qquad (3\text{-}40)$$

In order to represent the shell structure of atoms, we introduce a trial electronic potential $V^{shell}(r)$. Let $E_{n,l}$ a one-electron energy of (n,l) state with this potential. n and l mean the usual principal and azimuthal quantum numbers. We apply the Fermi-Dirac distribution for the electron population, the probability $P_{n,l}$ with which an electron is found in an (n,l) state is

$$p_{n,l} = \frac{2(2l+1)}{1+exp[(E_{n,l}+u)]} \qquad (3\text{-}41)$$

Here we suppose there are (2l+1) degenerate state for the up and down spin electrons. The number of bound electrons are written by the sum of $P_{n,l}$

$$N^b = \sum_{n,l} p_{n,l} \tag{3-42}$$

The number of free electrons N^f is calculated as follows. Since the minimum momentum of the free electrons at position r satisfies the equation

$$p_{min}{}^2/2m + eV = 0 , \tag{3-43}$$

the lower bound of the integration of Eq. (3-40) should start from $P_{min}(r)$. That is

$$N^f = \frac{1}{h^3}\int 4\pi r^2 dr \int_{p_{min}} \frac{8\pi p^2 dp}{1+exp[\beta(p^2/2m-eV+u)]} \tag{3-44}$$

Total electrons including free and bound ones is

$$N^{total} = N_b + N_f \tag{3-45}$$

If the V_{shell} is assumed to be **V**(r) whcih is obtained by the usual Thomas-Fermi models without separating the bound electrons from free, the condition (3-45) is not satisfied. The method to obtain a self-consistent V_{shell} and $E_{n,l}$ will be presented in the succeeding section, and we consider approximate solutions following the work by Zink [26].

Zink supposed two types of trial V_{shell}. One of them is a ion-sphere type potential. Let R_0 be a ion-sphere radius. The potential V_{shell} at r, which is not less than r_1 determined later, is the ion-sphere potential.

$$V_{shell} = \frac{Z^*}{R}\left(\frac{R}{r} + \frac{r^2}{2R} - \frac{3}{2}\right) \tag{3-46}$$

For $r<r_1$, V is taken to be

$$V_{shell} = \frac{Ze}{r(1+ar_2)} + \frac{Z^*}{R}\left(\frac{r}{2R_2} + A_1\right) \tag{3-47}$$

where A_1 is obtained from the continuity condition of the potential at r_1.

The charge neutrality condition requires that electrons of total charge Z be located inside R and makes a relation between r_1 and Z_*, i.e.,

$$A_1 = \frac{2ZAr_1}{(1+Ar_1)^2} - \frac{R}{r_1} + \frac{3}{2} \tag{3-48}$$

A is a parameter which is decided by a given Z.

Therefore, the potential V_{shell} is parametrized only by a single parameter Z^*. Z^* and plasma density is connected by the relation

$$Z^* = \frac{2ZAr_1}{(1+Ar_1)^3} + \frac{Z}{(1+Ar_1)^2} \tag{3-49}$$

The procedure of numerical calculation is as follows. First, value is set to an appropriate Z^* and we calculate the chemical potential u and r_1, A_1 from the Eq. (3-48). The obtained d is used to refine Z^*. Calculations are repeated till initial and obtained Z^* do not differ. Zink gave the pressure of the system as a function of temperature. One of his results is shown in Fig. 12 .The pressure obtained by Zink shows a certain jump at about ion density 15g/cm^3. He did not present the values of $E_{n,l}$ and we lack the informations about the detailed atomic structure obtained by this model. C.M.Lee$^{26)}$ added the contribution from the resonant state which is emerged in conntinuum states. He wrote the electron distribution as

$$n_e(r) = n_{free}(r) + n_b(r) + n_r(r)\,. \tag{3-50}$$

where n_r (r) is the elecron density of the resonant electron and derive from the resonant state distribution around a resonant energy $e^{l,re}$ of lth partial wave $\omega^{l}(e-e^{l,re})$ as

$$n_r\,(r) = \sum_{l}\sum_{m} \frac{e\omega^{l}(e-e^{l,re})de}{1+exp[b(e-u))]} \tag{3-51}$$

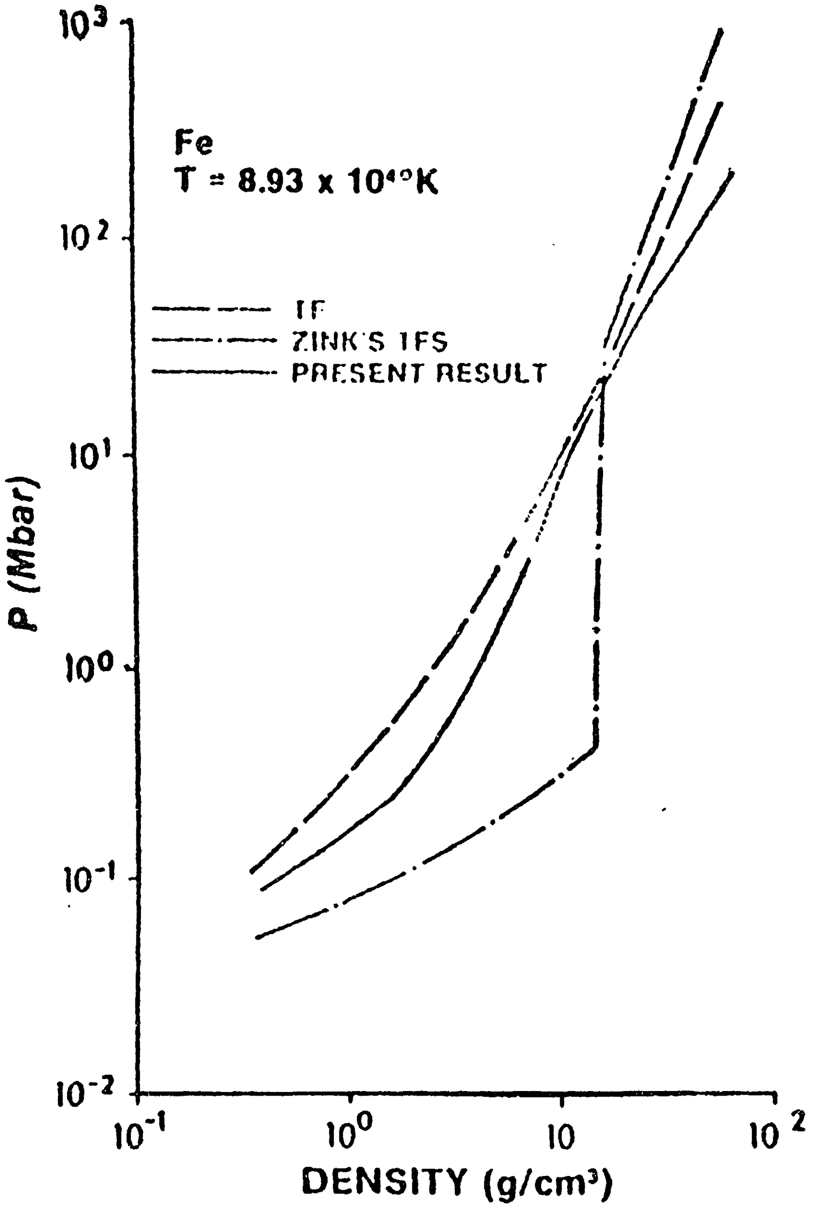

Fig. 12 Pressure against density calculated by Debye-Huckel models. (ref. 27)

The obtaind pressure (shown in Fig12 again) dose not jump and is smooth for the entire ion density.

IV Quantum Treatments

We treat electrons not as a classical particles but quantum ones in this section. The motion of the electrons is now expressed by the wave function. To obtain the wave function, we must set up an appropriate Hamiltonian. As is mentioned Introduction, there are many ways to do so. We can start with a single electron Hamiltonian or multielectron one, and we can use relativistic or non-relativistic, Hartree-Fock approximation or the Hartree-Fock-Slater approximatior Moreover, since the problem is quantum, there exist various methods of finding a solution such as the variational method, the perturbation method and the Green function method. The number of combination of the Hamiltonians, the approximations and the methods is almost infinite. Therefore, there is no single view point from which we can review the studies carried out by many researchers correlating each other. So we classify those works for that for a single atom and for atoms. A single atom problem is divided into multielecton and single electron problems.

IV-1 Atoms with External Field (Stark Broadening of Levels)

The earliest work which treats the Stark effect in plasma was that of Inglis and Teller[17]. They calculated level broadening and discussed the depression of series limit in emission spectra. This effect is one of the explanations of the experimental continuum lowering.

To discuss the Stark shift, the parabolic coordinate is suitable because the problem is not spherical symmetries. Following Inglis and Teller, let **F** be the external electric field. If N single charged ions are in a unit volume, the strength of the external field **F** is roughly written as

$$F = aeN^{2/3} \tag{4-1}$$

Holtzmark calculates a value to be 3.7. (This value is known to be the Holtzmark limit). With the given **F**, energy shift of n_0, n_1, n_2 (n_1, n_2 = 0,1,2,,,n-1) state is

$$\Delta E = (3/2)n_0(n_2-n_1)a_0eF\,, \tag{4-2}$$

where a_0 indicates the Bohr radius.
This shows that the maximum splitting of the energy of the n_0 orbital is

$$3n_0(n_0-1)a_0\,eF\,. \tag{4-3}$$

Since the energy of state n_0 is $1/2n^2$, the field **F** requireds to make the adjacent spectral lines of principal quantum number n and n-1 to be merged is

$$\frac{d}{dn}\,\frac{e^2}{2a_0n^2} = 3n_0(n_0-1)a_0eF\,, \tag{4-4}$$

$$F = e/[3a_0^2n_0^4(n_0-1)] \quad \approx \quad e/3a_0{}^2n_0{}^5$$

Using Eq. 4-4, we can obtain a rough estimation of the density at which the line of state n merges into the continuum.

$$3.7eN^{2/3} = \frac{e}{3a_0^{\,2}\, n_0^{\,5}} \,,\; N = (11.1\, a_0^{\,2} n_0^{\,5})^{3/2} \tag{4-5}$$

Yamamoto and Narumi[23) have recently calculated the energy shift of a hydrogenic neon caused by to the external electric field from neighbouring ions.

They wrote the potential in multipole expansion,

$$V(r,R) = -\frac{Z}{r} - Z_p \cdot \sum_{l=0} \frac{r^l}{r^{l+1}} P_l(cos(0)) \tag{4-6}$$

where Z_ρ and R represent the charge and the position of a perturber, respectively.

Using this expression, they write the eigen value of the bound Stark state as,

$$E_{n,n_1,n_2} = -\frac{Z^2e^2}{2n^2a_0} - \frac{3}{2}(n_1-n_2)\frac{1}{Zn^3}\frac{e^2Z_p}{a_0}\varepsilon^2$$

$$-\frac{1}{2}\frac{[6(n_1-n_2)^2-n^2+1]n^2}{Z^2n^4}\frac{e^2z_i}{a_0^{hw}}\varepsilon^3 \tag{4-7}$$

where $e=n^2a_0/R$

The second term corresponds to the linear Stark profile and the third to the quadrupole correction. From Eq. 4-7, shift of Lyman-series $\Delta\omega_k{}^d$ can be calculated as

$$\Delta w_K{}^d(\beta) = \frac{3}{2}F\frac{ea_o}{\hbar Z}\Delta_k^d \tag{4-8}$$

where $\Delta_k{}^d$ is defined by

$$\Delta_k^d = -n(n_1-n_2)+n'(n'_1-n'_2) \tag{4-9}$$

and $\mathbf{F}$ means the strength of the electric field (eZ_p/R^2). Applying electric microfield distribution for $\mathbf{F}$, they obtained the Stark profile. Numerical values of the halfline width are tabulated in their original paper. Figure 13 shows broadening of levels, which is superposed on the energy shift caused by the screening effect discussed in subsection II-2. (see Fig. 9)

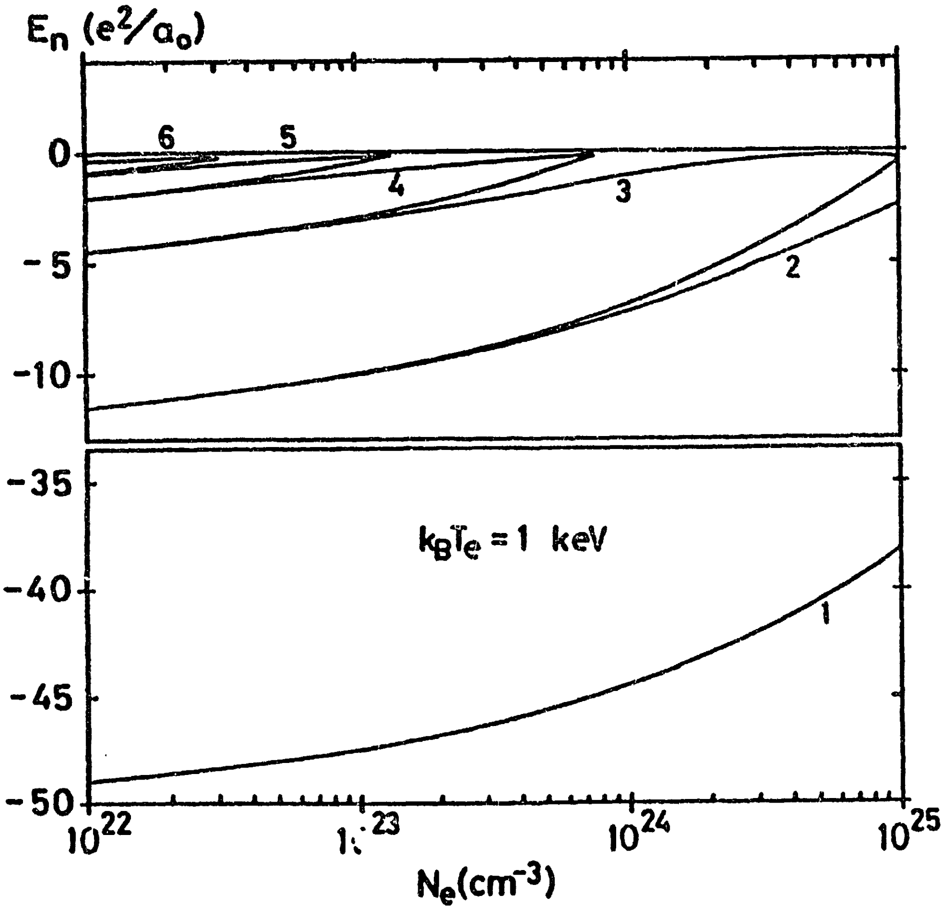

Fig. 13 Energy levels broadened by Stark shift for a hydrogenic Neon. (ref. 9)

IV-2 Average Atom Model and Quantum Cell Model

In the preceding subsections, we have considered a single electron orbital of an atom in a given model potential in section II. Now we go into the multi-electron problem.

Let's consider an atomic state of a particular ith atom in plasma. In real plasma, the atomic state . i.e., the electronic configuration, charge state distibution, and the energy of orbitals and so on can be specified definitely. However, we are interested in quantities averaged over the atoms in plasma, e.g., the average degree of ionization, the energy or the electron occupation number of orbitals. To obtain these values, we must calculate the electronic state of each atom which is interacting each other and then take the average of these physical quantities. This procedure needs a lot of calculation. But, if the atoms are in thermal equiribrium, we can solve the problem much easier by introducing a hypothetical average atom which has the following characteristics.

1) The electron occupation number P(n,l) of the n,l bound orbit is not necessarily be integer, thought a real atom in plasma has integer occupation numbers.

2) P(n,l) satisfies the Fermi-Dirac distribution.

We suppose all the electronic properties of the plasma are derived from the characteristics of this atom. Though the justification of this assumption may not be clear, this hypothetical atom (often called an Average Atom) is frequently discussed as a representative of the atoms in the plasma for its simplicity. In order to calculate the energy levels of the average atom, we can utilize a variety of the methods which are familiar in quantum mechanics. One of them is the Hartree-Fock approximation.

Let $R_{n,l}$ be the radial wavefunction of a bound state in the effective potential V_{eff}. $R_{n,l}$ satisfies the Shroedinger eq.

$$-\frac{1}{r^2}\frac{d}{dr}[r\frac{d}{dr}R_{n.l}(r)]+[\frac{2l(l+1)}{r_2}+V_{eff}]R_{n,l}=\varepsilon_b R_{n,l} \qquad (4-10)$$

Then the radial density of bound electron for the average atom is written as

$$n_b(r) = \frac{1}{4\pi} \sum_{n,l} \frac{2(2l+1)}{1+exp([\beta(E_{n,l}-\mu)]} \left| \frac{R_{n,l}(r)}{r} \right|^2 \tag{4-11}$$

where n,l summation runs over all the bound states.

For the density of free electron $n_f(r)$, the Thomas-Fermi or the Thomas-Fermi-Dirac approximation is applicable. In the case of the TF model, $n_f(r)$ is expressed as

$$n_f(r) = \int_{p_0}^{\infty} \frac{p^2 dp}{1+exp[\beta(p^2/2m+V_{eff}-\mu)]} \tag{4-12}$$

The effective potential V_{eff} is common to all the bound electrons and written as the sum of the attractive Coulomb potential by nuclus and the repulsive and exchange potentials between electrons and correlation if needed, i.e.,

$$V_{eff} = -\frac{Ze^2}{r} + V_c(r) + V_{ex}(r) + V_{corr}(r) + [V_i(r)] \tag{4-13}$$

where $V_i(r)$ stands for the potential caused by surrounding ions.

The present setting of the problem gives the results of an isolated atom. The **Average Atom** correctly represents the features of the atom in plasma only if effective potential V_{eff} reflects the plasma properties or an correct boundary condition on wavefuntion is applied.

There are two types of boundary conditions for the average atom model.

Type I

The wavefunction of the type I average atom is zero at infinity. In this case effective potential V_{eff} reflects the contribution from the ions in plasma and satisfies the condition,

$$\begin{aligned} V_{eff}(r) &= 0 \\ V_{eff}(r) &= -eZ/e' \end{aligned} \qquad (4\text{-}14)$$

There are various ways to take into account the contribution from the ions. For example, we can assume V_{eff} to be Debye-Huckel type, that is, the distribution of ions $n^i(r)$ is given by the Maxwell-Boltzmann distribution,

$$n_i(r) = e^{-\beta Z_i V_{eff}}$$

One of the difficulties with the type I average atom model is concerned with the self-consistency between the obtained wavefunctions and the initial assumed effective potential. We can not expect that all of the solutions of eq. 4-10 are real wavefunctions, because, as is mentioned in the introduction, they may have a large amplitude at the position of the other ions. This difficulty becomes more apparent when ion density goes higher. In order to get rid of this undesirable result, the Fermi-distribution 4-11 can be modified and $n_b(r)$ is replaced by a phenomenological parameter D^n,

$$D_n = 2n^2/(1+a(r_0^n/R_0)^b), \qquad (4\text{-}15)$$

where R_0 and the $r_0{}^n$ are the ion-sphere and radius of the n-th shell of a neutral atom. By choosing appropriate values for a and b in eq. 4-15, number of bound states is limited since the delocalized orbital changes its nature into that of continuum states.

Type II

The second one is the ion-sphere type boundary condition. The wavefunction of the bound electron should be confined inside the ion-sphere defined by R_0. This can be done by putting the boundary condition of radial wavefunction as

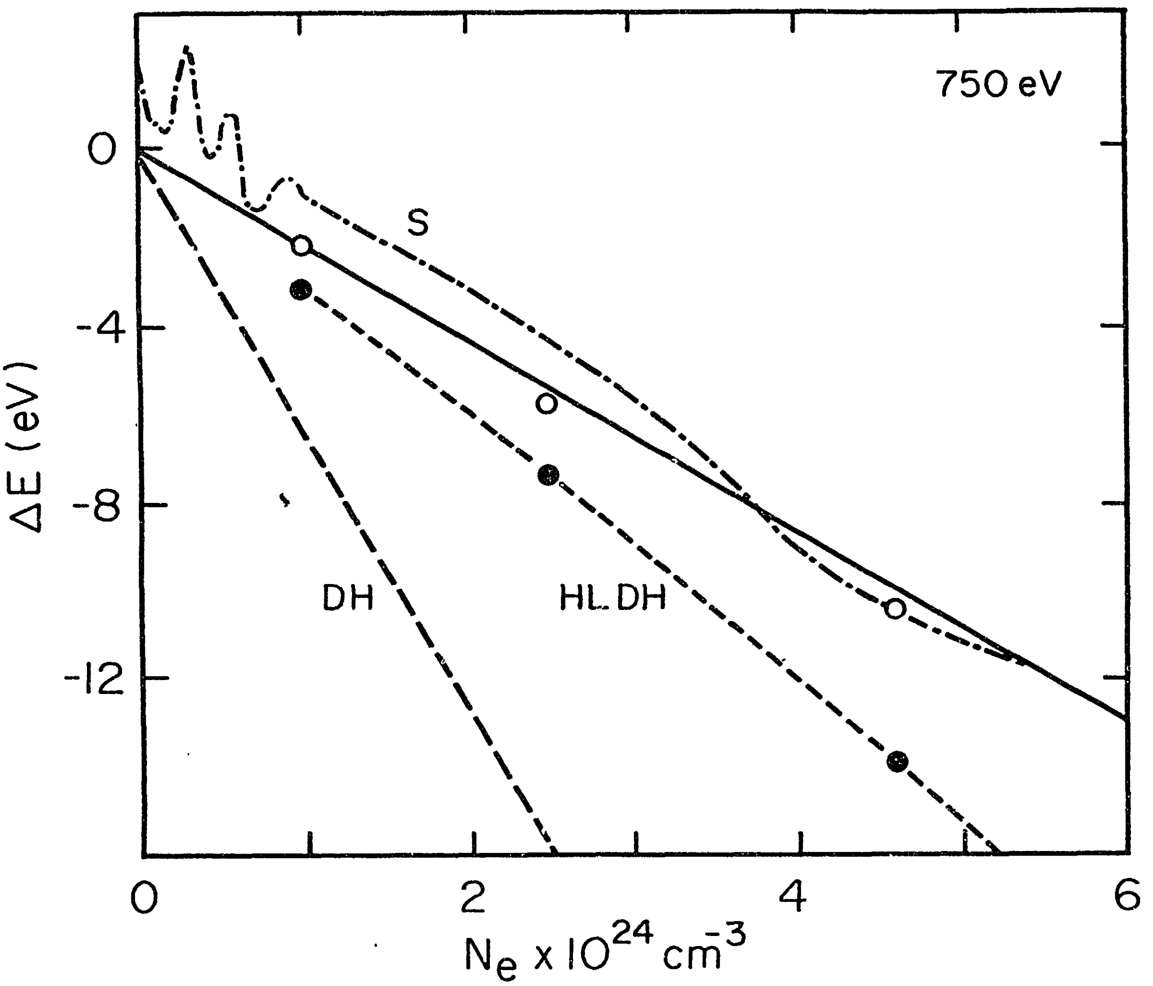

Fig. 14 Lyman α line shift of Neon impurity in a dense plasma at T_e = 750 eV. [IPPJ-AM-31, Institute of Plasma Physics, Nagoya University, Japan (1983)]

$$R_{n,l}(0) = 0$$

$$R_{n,l}(r_0) = 0 \quad or$$

$$\frac{d}{dr}\left[\frac{R_{n,l}(r)}{r}\right] = 0 \quad at \quad r = R_0 \tag{4-16}$$

$R_{n,l}$ is normalized as

$$4\pi\int_0^{R_0} r^2 R_{n,l}{}^2(r)\,dr = 1 \tag{4-17}$$

Since the contribution from other ions is represented by the ion-sphere boundary condition, $V_i(r)$ needs not be added to $\mathbf{V}_{eff}$. The average atom model with this type of boundary condition is often called the **Quantum Cell Model.**

S. Skupsky discussed the X-ray line shift of hydrogenic Neon based on type I boundary condition. One of his typical results is shown in fig 14 . The shift of 2p - 1s transition energy oscillates at low electron density region. On the contrary to the results of ion-sphere model discussed in subsection III-2 , blue shift can be expected at particularly density regions.

B. Rozsnyai [18)] worked with the boundary condition of type II. In his work Iron atom was investigated taking into account the relativistic effect. There are many figures and tables in his original paper.

IV-3 Cluster Calculation Approaches

The binding nature between ions in plasmas can be taken account if cluster or molecular calculation is applied to investigate the electronic properties of plasmas. Since most cluster calculation need larger computational effort than single atom calculation, there are only a few examples. One of them is the Discrete Variationa X_α (DV-X_α) mehtod.

Though ions move randomly in plasmas, the DV-Xa method deals with fictitious cluster in which atomic configuration is fixed. The physical background of the model is based on the discussion that the configuration of ions becomes a spatial closest pack at a high-density limit. So,this model is applicable for high G plasmas. The ion density can be controled by changing the interatomic distances in the cluster. By applying the Fermi-Dirac distribution for electron occupation, the effect of electron temperature can be simulated. In the DV-X_α method, single electron states are calculated on the basis of effective potentials which involves the exchange interaction between electrons in an approximate form of the local potential. The local potential is expressed as being proportional to the cubic root of the local density n(r) at each point. The total Hamiltonian of the cluster is given by

$$H = - \sum_{i=1}^{N} \nabla_i^2 + U_c + U_{ex}$$

where N is the number of electrons in the cluster and U^c is a Coulomb potential term and U^{ex} represents an exchange interaction term in atomic units. The wavefunction Ψ of the cluster is written by the superposition of the atomic orbital (LCAO-MO) and expressed as

$$\Psi = \sum_j C_j X_j$$

where X^j is symmetrized orbitals. With the Hamiltonian and overlap matrices $H^{i,j}$ and $S^{i,j}$, given by

$$H_{i,j} = <X_i|H|X_j>, \quad S_{ij} = <X_i|\ X_j>$$

the secular equation for C is

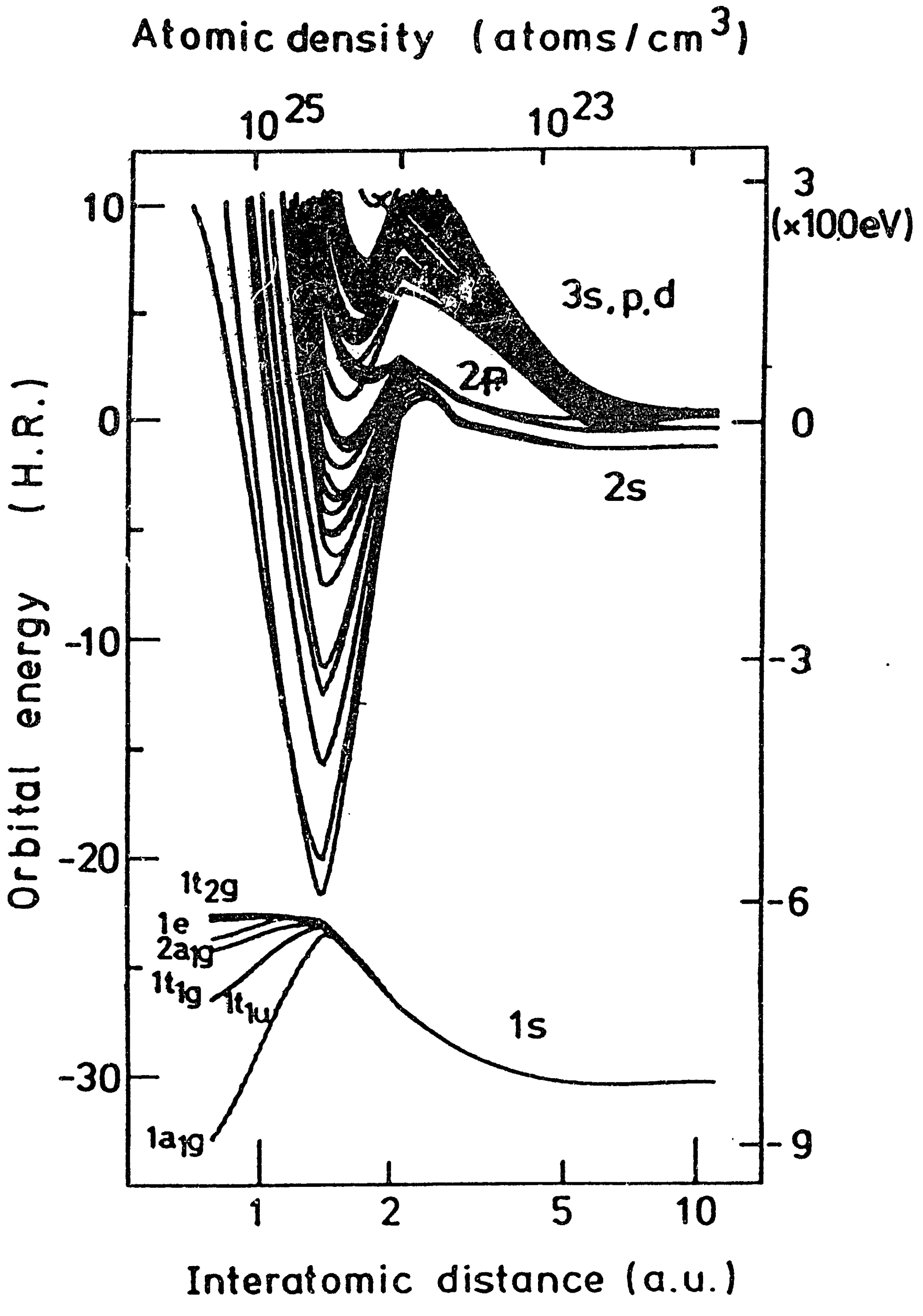

Fig. 15 Orbital energies for face-centered-cubic cluster Ne_{13} against the nearest-neighbor atoms. (ref. 28)

$$HC = \varepsilon SC$$

where represents the energies of orbitals. The charge neutrality condition decides the boundary condition of the wavefunction.

The electron occupies each orbital with Fermi-Dirac distribution; that is

$$P_k = a_k \frac{1}{1 + exp(\beta(\varepsilon_k - \mu))}$$

The calculation is repeated till the self-consistency is achieved between the resultant wavefunctions and trial charge distribution.

One of their results at zero temperature is given in the Fig.15., which shows that one electron energies are given as a function of interneuclear distance for the face-centered cubic Ne13 clusters. For the simple cubic Ne8 cluster, the energy diagram is not different appreciably from that of Ne13.

The 2s and 2p orbitals form band-like structure and broaden their energy levels, which can represent the so-called continuum lowering. The core 1s orbital gains energy with decreasing internueclear distance in the region of 10~2 a.u., because the screening charge of the nuclear attractive potential increases. At an extremely high density region (higher than 3×10^{23} atoms/cm^3), kinetic energy of electrons rapidly increases because they are confined in a small limited volume. The increase in kinetic energy of outer shell electrons is also seen in the region around 10^{24} atoms/cm^3 ; this corresponds to the pressure ionization. Within the fictitious cluster, the effective potential for one-electron orbital, which is same for all orbitals in the DV-Xαmodel, change its nature from the Coulombic to highly screened potential as is seen in fig. 16 .

When electron temperature goes up with fixed ion density, the mixing of the atomic wavefunctions between neighboring atoms becomes less important. This is one of the natural demonstrations that atomic representation of the electronic property holds valid in high temperature plasma. Since thermally ionized electron forms almost uniform charge distribution, the screening charge of attractive core potential becomes small. Then, the core orbitals comes to be bounded more tightly and sequentially the overlap of

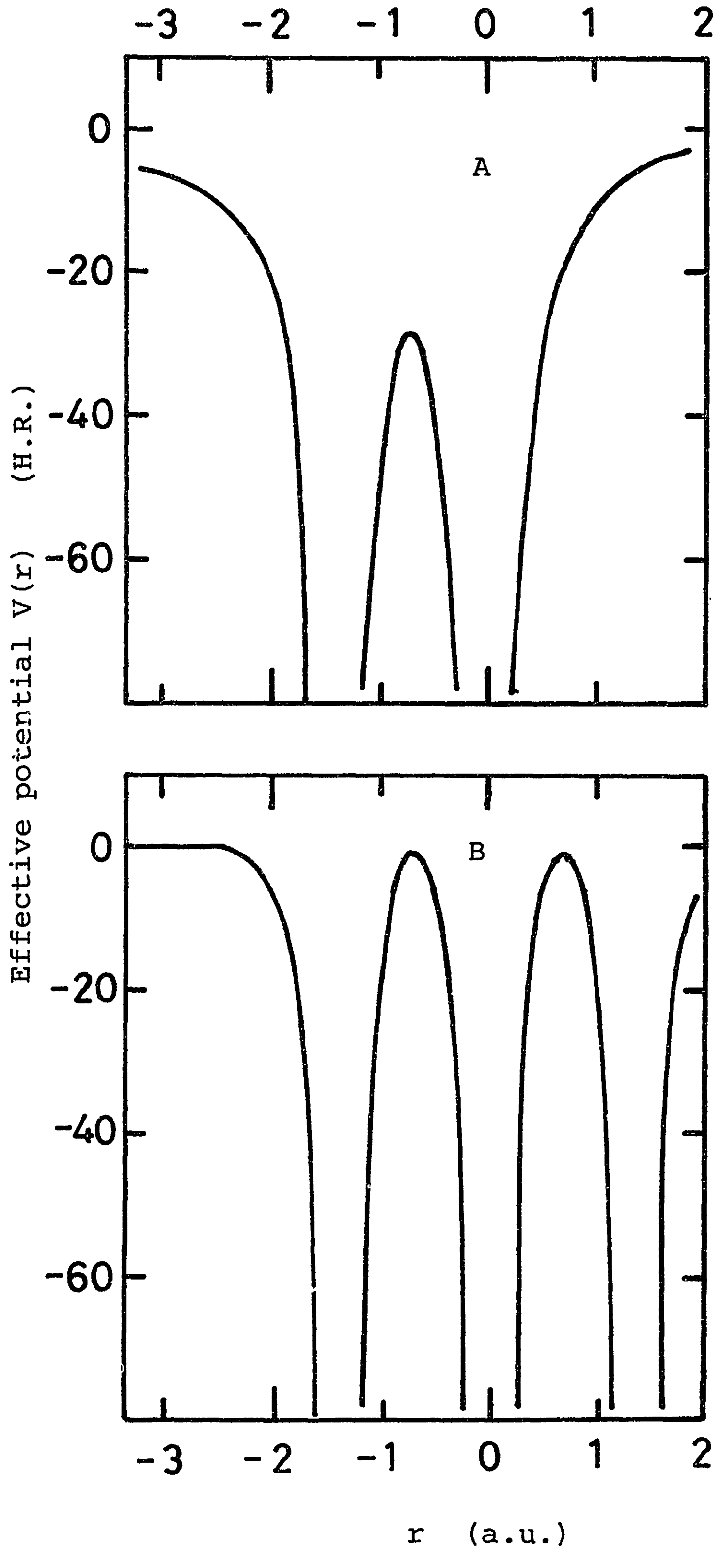

Fig. 16 Effective potentials at different electron densities.

the wavefunction becomes small. This feature is illustrated in Fig. 17.

Recently this method has been applied to the analysis of the X-ray emission spectra (shown in Fig. 1) of Si which is in grass micro balloon target in the inertial confinement fusion experiment. The density and electron temperature for the spectrum shown in fig. 1. are estimated to be 10g/cm^3 and 200 eV, respectively.

Since the Lyman series of Si^{+13} can be clearly seen in the spectrum, the electronic configuration of the emitter atom dose not differ much from those of isolated Si-ion. So a photo emitter Si ion in a model cluser is is surrounded by eight Si atoms with the average electronic configuration in the plasma. LCAO-MO wavefunctions are used for the bound state. The free electron distribution was computed using the Thomas-Fermi method. The Fermi-Dirac distribution is used to get the occupation number of the orbital for surrounding eight atoms. By inverse-transforming the LCAO-MO to Atomic Orbital, the central Si atom can keep hydrogenic configuration within the MO-picture. Numerical basis functions 1s to 5f of Si atom are used for the calculation.

The obtained X-ray transition energies from np to 1s are plotted in the fig.1 again. In these calculation electron temperature is supposed to be 200 eV and ion densities are 4, 8, 12, 20, and 40 g/cm^3. Transition energies are not indicated If the initial orbital np mixed with the orbitals of neighboring ions and loses atomic property.

The calculated spectra differ from that of isolated Si^{+13}. Firstly, transition energy 2p - 1s shifted red-side about 15 eV when ion density goes to 40g/cm^3. Secondly, 3p level splits into 2 or 3 lines at the density 8 - 12 g/cm^3. The transition from 3p to 1s at 8g/cm^3 is not observed experimentally. From these facts we think emission lines 2p - 1s and 3p -1s from Si atom in high density and temperature plasma is not observed as sharp lines but as broad peaks. Since the 4p and 5p orbitals are mixed with those of neighboring Si atoms , the transition from those orbitals are burried into the continuum.

The merit of the cluster calculation is summarized in th following points. If a single ion is taken as a representative of ions in plasma, it is difficult to find an appropriate boundary

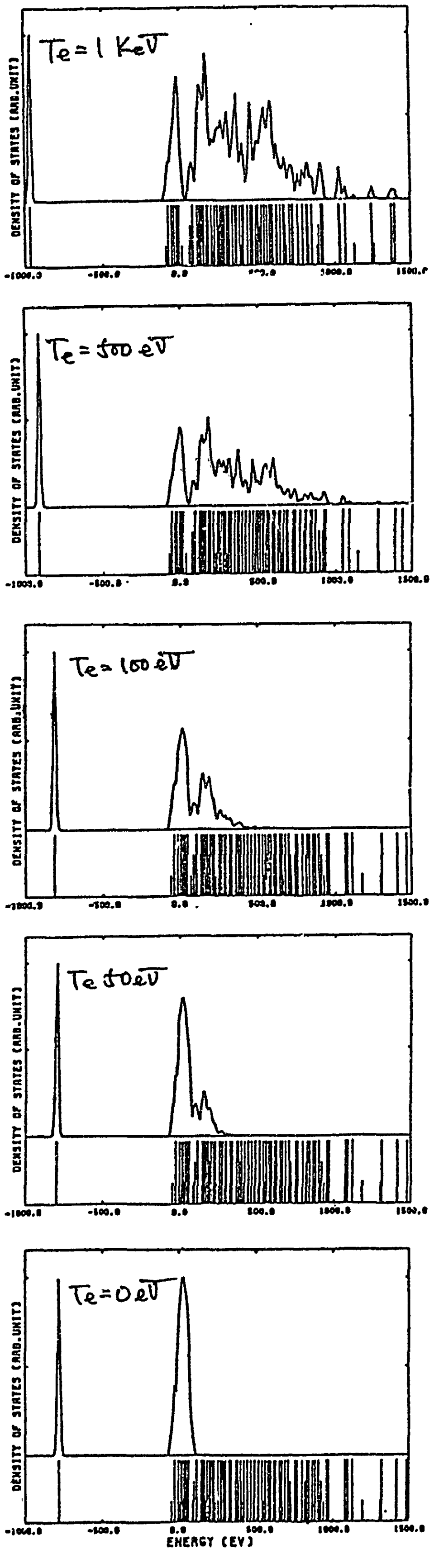

Fig. 17 Density states of condensed Neon clusters at various temperature. Energy positions calculated are shown at the lower part of figures.

conditions for wavefunction as seen in sub-section IV-2. With the cluster calculation, the boundary condition of the wavefunction becomes less important when the size of cluster becomes large. For example the wavefunction located at the central atom of the cluster can be represented much easier without thinking about its boundary condition provided a realistic atomic configuration around the ion is given. And also the contribution of surface energy to the total energy of the cluster, which depends on the choice of Hamiltonian and boundary condition of cluster, becomes small for a huge cluster. However, this extention of cluser size requires a bigger computational effort.

IV-3-b Cluster model calculation using extended Huckel method

Collins and Merts calculated electronic properties of clusters which contain about 100 atoms using the extended Huckel method. Their calculation is based on the Born-Oppenheimer approximation, namely fixed atomic configuration as DV-X_α method mentioned in the above subsection. The band width of Na, Al Ccu and Fe are calculated as a function of interatomic separation or in other word, compression in the range of ion density from 10^{23} to 10^{26}. The electron temperature is supposed to be zero and the thermal motion of ions is not directly taken into account in their calculation. However, one of their important results is that the distortion of atomic configuration by the thermal motion of ions will change the band width by at most 10 % at the temperature below 500 K and the mixing of atomic orbital has a large contribution to the broadening of levels at the plasma parameters they are investigated.

V Conclusion

At the beginning of this article, we started our discussion with the reasonablly genral description of the problem. We wrote a time dependent Hamiltonian o the system consist of nucleus and electrons and showed how it can be reduced into atomic models in plasmas. Though a lot of fruitful results have been achieved using these method and they can explain the experimental results fairly well, authors of this article think the present study on atomic problem in plasma is not adequate.

For example the broadening of level is expalined in different way atomic an molecular models, In the atomic picture, the level broadening is acumulation of energy shifts of he orbitals, i.e., tim averaging of energy shift. If we evaluate the electronic propertis of plasmas in time, we can get a perturbed potential at a given time. This perturbation potential will cause the shift of energy and the distribution of energy levels as a function of time is related to the broadening of the levels if we take the atomic picture. The effective potential models fo a ion in plasmas calculate the shift of energy but they are not directly connected to this time averaging procedure or at least their relation is not clear. On the contraly, the molecular calculation shows the broadening of levels even if ions do not move, namel T=0. The width of levels by melecular calculation should be enhanced by the thermal motion of ions. These two models are valid at different plasma marameters, however, they should be combined. The key to this goal seems to be the time evaluation of plasmas.

An urgent requirment for theoretical study of atomic processes in plasmas is getting information usuful for designing a nuclear fusion reactor, that is how we get much more high compression and high temperature in inertial confinement fusion. Speaking more concretely we have to answer the question such as how do electron and ion become hot at shock front and how does radiation transport the energy in the course of compression.

Again we feel a need for a time dependent calculation of atomic properties in plasmas. However, at present, non of models in this article can not predict the behaviour of electrons and ions because the motion of ions is thoughly omitted from the discussions. Only a few model seems to be able to describe the properties of atoms in real plasmas with some future extension of theories. These extensions are realy desired not only for the progress of ICF program but also for the basis study of UV and X-ray lasers and so on.

Acknowledgement

Authors would like to express their thanks to Prof. K.Mima of Institute of Laser Enginnering, Osaka Univ., Prof. K. Yonei and H. Toutsuji in Okayama Univ., for their helpful discussion. K.F. expresses special thanks to Prof. T. Fujimoto of Kyoto Univ. for careful reading of the manuscript and Prof. T.Watanabe for continuous encouragement.

This work is partly supported by as a joint program of Research Information Center in the Institute of Plasma Physics, Nagoya Univ.

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