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RESEARCH REPORT

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Abstract

Calculations based on a variational method with wave functions including the correlation of electrons are carried out to obtain energy eigenvalues of Schrödinger's equation for helium-like atoms embedded in dense plasmas, taking the Debye-Hückel approximation. Energy eigenvalues for the 1^1S, 2^1S, and 2^3S states are obtained as a function of Debye screening length.

Numerous authors[1-10] in the past have attempted to find solutions of Schrödinger's equation for an electron in a screened Coulomb potential. However, there is no research of energy eigenvalue for a two-electron system in dense plasmas. In this paper, we are interested particularly in the 1^1S, 2^1S and 2^3S bound states of helium-like atoms embedded in dense plasmas. In order to find the energy eigenvalues of these states, we take the Debye-Hückel approximation which has been used in several fields of physics. Although the Debye-Hückel model is a good approximation for low density and high temperature plasmas, it has been examined over a wide range of the plasma conditions. We employ two models describing the electron-electron interaction to simplify the calculations; one is to assume no screening and the other is to assume the same screening of Debye-Hückel type as the nuclear charge. We consider that these two cases show the extreme values of complete screening and no screening, and the correct values must lie between the two cases. Using perimetric coordinates used by Pekeris[11-13] for S states of the two-electron atoms, a variational method is developed to obtain solutions of Schrödinger's equation for Hamiltonian of the above model. We employ atomic units in this paper.

The Schrödinger's wave equation of the problem is given as

$$\left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + 2\frac{\partial^2}{\partial r_{12}^2} + \frac{4}{r_{12}}\frac{\partial}{\partial r_{12}} + \frac{r_1^2-r_2^2+r_{12}^2}{r_1 r_{12}}\frac{\partial^2}{\partial r_1 \partial r_{12}} \right.$$

$$\left. + \frac{r_2^2-r_1^2+r_{12}^2}{r_2 r_{12}}\frac{\partial^2}{\partial r_2 \partial r_{12}} + 2\left(E + \frac{Z}{r_1} e^{-\frac{r_1}{D}} + \frac{Z}{r_2} e^{-\frac{r_2}{D}} - \frac{1}{r_{12}} e^{-\frac{r_{12}}{D}}\right)\right] \Psi(r_1, r_2, r_3) = 0, \quad (1)$$

where r_1 and r_2 denote the distances of electrons from nucleus, r_{12} the distance between two electrons, E the energy eigenvalue, Z the atomic number, D the Debye screening length, and $\Psi(r_1,r_2,r_{12})$ wave function for S states. We calculated the energy eigenvalues for two cases of $D_{12}=\infty$ and $D_{12}=D$ as the electron-electron interaction. Transformating by perimetric co-ordinates $u = Z(-r_1+r_2+r_{12})$, $v = Z(r_1-r_2+r_{12})$, $w = 2Z(r_1+r_2-r_{12})$, and taking

$$\Psi(u,v,w) = \exp\{-\frac{1}{2}(u+v+w)\}F(u,v,w), \text{ we have that}$$

$$\exp\{-\frac{1}{2}(u+v+w)\}\{ G_1\frac{\partial^2}{\partial u^2}+G_2\frac{\partial^2}{\partial v^2}+G_3\frac{\partial^2}{\partial w^2}+G_4\frac{\partial^2}{\partial u\partial w}+G_5\frac{\partial^2}{\partial v\partial w}+G_u\frac{\partial}{\partial u}$$
$$+G_v\frac{\partial}{\partial v}+G_w\frac{\partial}{\partial w} + (G_{61}-\lambda G_{62} + \frac{E}{2Z^2}G_{63})\} F(u,v,w) = 0, \qquad (2)$$

where
$$G_1 = 4u^2v + 4uv^2 + 4u^2w + 4uvw + 2uw^2 ,$$

$$G_2 = 4uv^2 + 4u^2v + 4v^2w + 4uvw + 2vw^2 ,$$

$$G_3 = 8u^2w + 8v^2w + 4uw^2 + 4vw^2 ,$$

$$G_4 = -8u^2w - 4uw^2 ,$$

$$G_5 = -8v^2w - 4vw^2 ,$$

$$G_u = -4u^2+4v^2 + 8uv + 4uw + 4vw + 2w^2-4u^2v-4uv^2-4uvw ,$$

$$G_v = 4u^2-4v^2 + 8uv + 4uw + 4vw + 2w^2-4u^2v-4uv^2-4uvw ,$$

$$G_w = 8u^2 + 8v^2 - 4w^2 - 4u^2w - 4v^2w - 2vw^2 - 2uw^2 ,$$

$$G_{61}= \frac{1}{2} G_{63}- (4u^2 +4uv +2uw +2vw)(1-e^{-\alpha(2v+w)})$$
$$- (4v^2 +4uv +2vw +2uw)(1-e^{-\alpha(2u+w)}) ,$$

$$G_{62} = (4uv + 2uw + 2vw + w^2) e^{-2\alpha_{12}(u+v)} ,$$

$$G_{63} = 4u^2v + 4uv^2 + 2u^2w + 2v^2w + 4uvw + uw^2 + vw^2 ,$$

$$\alpha = 1 / 4ZD , \qquad \alpha_{12} = 1 / 4ZD_{12} ,$$

$$\lambda = 1 / Z .$$

In order to solve eq.(2) by the variational method, we consider the following variational wave function,

$$F(u,v,w) = \sum_{l,m,n} A(l,m,n) (u^l v^m \pm u^m v^l) w^n , \tag{3}$$

where the coefficients A(l,m,n) denote linear variational parameters, + the singlet state and - the triplet state. By the use of the variational wave function (3), we obtain the following secular equation,

$$\left| \Delta(l,m,n;l',m',n') + \lambda A(l,m,n;l',m',n') - \frac{E}{2Z^2} B(l,m,n;l',m',n') \right| = 0, \tag{4}$$

where $\Delta(l,m,n;l',m',n') = \frac{1}{2}\{ \Delta_1(l,m,n;l',m',n') + \Delta_1(l',m',n';l,m,n)\}$

$$-\frac{1}{2}\{G_{61}(l,m,n;l',m',n') + G_{61}(l',m',n';l,m,n)\},$$

$$A(l,m,n;l',m',n') = \frac{1}{2}\{G_{62}(l,m,n;l',m',n') + G_{62}(l',m',n';l,m,n)\},$$

$$B(l,m,n;l',m',n') = \frac{1}{2}\{G_{63}(l,m,n;l',m',n') + G_{63}(l',m',n';l,m,n)\}.$$

All integrals of $\Delta_1(l,m,n;l',m',n')$, $G_{61}(l,m,n;l',m',n')$, $G_{62}(l,m,n;l',m',n')$ and $G_{63}(l,m,n;l',m',n')$ are expressed with a formular

$$K_n(\xi) = \int_0^\infty x^n e^{-\xi x} dx = n! \xi^{-(n+1)}.$$

From the use of secular equation (4), we studied energy values with respect to Debye screening lengths and critical Debye screening lengths D_c, where the energy eigenvalues become zero, of the 1^1S, 2^1S and 2^3S states of helium atom in dense plasmas for two cases of $D_{12} = \infty$ and $D_{12} = D$. We calculated the energy values for several values of the total number of linear variational parameter(N). We confirmed that the case of N=444 is sufficient to get energy values with five or six figures at low density ($D^{-1}<0.5$). The present results of energy eigenvalues for the 1^1S, 2^1S and 2^3S states in the case of N = 444 are given for two cases of $D_{12}=\infty$ and $D_{12}= D$ in Table I. The energy eigenvalues for the D^{-1} values greater than 0.6 in the case of $D_{12}=\infty$ were calculated with N=525. It is noted that the energy levels of the 2^3S state are lower than those of the 1^1S for $D^{-1}>0.8$. Extrapolating the values of the energy near zero, we determined the critical Debye screening length D_c for the zero energy eigenvalue in the case of $D_{12}=D$. The critical Debye screening lengths for the 1^1S, 2^3S and 2^1S states were found to be 0.4498, 0.4890 and 0.5068, respectively, for the case of $D_{12}=D$. Energy separation between neighbouring states decreases as seen from the table when the screening length increases. It is seen that no bound state exists in the high-density limit.

The energy values for helium-like ions can be also calculated by the same method. The scaled total energies E/Z^2 are plotted in Figs. 1, 2 and 3 for the helium atom, oxygen ion (O VII) and iron ion (Fe XXV) as a function of scaled Debye screening length DZ. We also plotted the energy values of hydrogen-like ions from Rogers et al.[6] by the dot-dashed lines. The solid lines and the dashed lines indicate the results for $D_{12} = \infty$ and $D_{12} = D$, respectively.

The total energy of the 2^1S state for He I coincides with that of the 1^1S state of He II at DZ = 20 (for $D_{12} = \infty$) and 8 (for $D_{12} = D$) as shown in Fig.1. This means that the 2^1S state in He I is ionized to He II at this point. For the ground state 1^1S of He I, the pressure ionization occures at DZ = 2 for $D_{12} = \infty$ but not happened for $D_{12}=D$. The same curves for O VII and Fe XXV are shown for the 1^1S, 2^1S and 3^1S states in Figs. 2 and 3. For the excited states 2^1S and 3^1S , the difference between the results with $D_{12} = \infty$ and $D_{12} = D$ is less than 2% for DZ > 3. The cross points of the excited states 3^1S and 2^1S with hydrogen-like ground state for O VII are DZ = 10 and 4.5 , respectively. The cross point in the scaled value of DZ decreases when the nuclear charge Z increases. When Z increases, the difference between $D_{12}=\infty$ and $D_{12}=D$ decreases. For Fe XXV, the difference between the two cases is within 5% for DZ>2.

Generally, the Debye-Hückel model is valid for high temperature and low density plasmas; the ion-coupling parameter $\Gamma = (Z^*e)^2/R_0kT_e < 1$. Here Z^* is the effective charge and $R_0 = (3Z^*/4\pi n_e)^{1/3}$ is the average ion distance, and Γ is given as

$$\Gamma = (4\pi n_e/3Z^*)^{1/3}(Z^*e)^2/kT_e.$$

The Debye screening length is written as

$$D = (4\pi(Z^*+1)e^2n_e/kT_e)^{-1/2}.$$

Then Γ is expressed by n_e or T_e as

$$\Gamma = \frac{2.15\times10^{2}\ Z^{*5/3}\ (Z^{*}+1)}{(DZ)^{2}\ [n_e(10^{20}cm^{-3})]^{2/3}} ,$$

or

$$\Gamma = \frac{6.3\ Z^{*5/3}\ (Z^{*}+1)^{1/3}}{(DZ)^{2/3}[T_e(eV)]^{2/3}} .$$

The values of Γ are plotted in Fig.4 as a function of DZ for $Z = 2$ ($Z^{*} = 1$) and $Z = 8$ ($Z^{*} = 7$). Fig. 4 shows that the region of $n_e<10^{24}cm^{-3}$ and $T_e>20eV$ gives $\Gamma <1$ and this region corresponds to that of DZ>1 for Z=2. We have $\Gamma <1$ at DZ>1 when $T_e>5keV$ and $n_e<10^{27}cm^{-3}$ for Z=8. Then the plasma condition at DZ=1 is not so far from the validity region for the Debye-Hüchel model for Z<8. But for Z=26, the condition of $\Gamma <1$ at DZ≈1 needs the plasma parameters of $T_e>100keV$ and $n_e\approx10^{29}cm^{-3}$. For the regions of T_e=20keV and $n_e\approx10^{26}cm^{-3}$, DZ=10 is derived. It is considered that the Debye-Hüchel model is appropriate at DZ>10 for Z=26.

The calculation was carried out by use of the FACOM computer at the Institute of Plasma Physics in Nagoya University.

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Table I. Energy eigenvalues for the 1^1S, 2^3S and 2^1S states of helium atom in dense plasma.

	1^1S		2^3S		2^1S	
D^{-1}	$D_{12}= D$	$D_{12}= \infty$	$D_{12}= D$	$D_{12}= \infty$	$D_{12}=D$	$D_{12}= \infty$
0.00	-2.90372	-2.90372	-2.1752	-2.1752	-2.1460	-2.1460
0.05	-2.75655	-2.7083	-2.0320	-1.9872	-2.0037	-1.9597
0.10	-2.61485	-2.5216	-1.9010	-1.8210	-1.8750	-1.7983
0.20	-2.34700	-2.1723	-1.6703	-1.5509	-1.6509	-1.5421
0.40	-1.86845	-1.5644	-1.3039	-1.1954	-1.2959	-1.1879
0.60	-1.45856	-1.0635	-1.0168	-0.9154	-1.0116	-0.9069
0.80	-1.11033	-0.679	-0.7770	-0.663	-0.7720	-0.663
1.00	-0.81821	-0.476	-0.5747	-0.483	-0.5694	-0.398
1.25	-0.52495	-0.270	-0.3685	-0.278	-0.3622	-0.187
1.50	-0.30421	-0.110	-0.2091	-0.119	-0.2008	-0.026
1.75	-0.14874	------	-0.0917	-0.001	-0.0794	------
2.00	-0.05034	------	-0.0111	------	-------	------

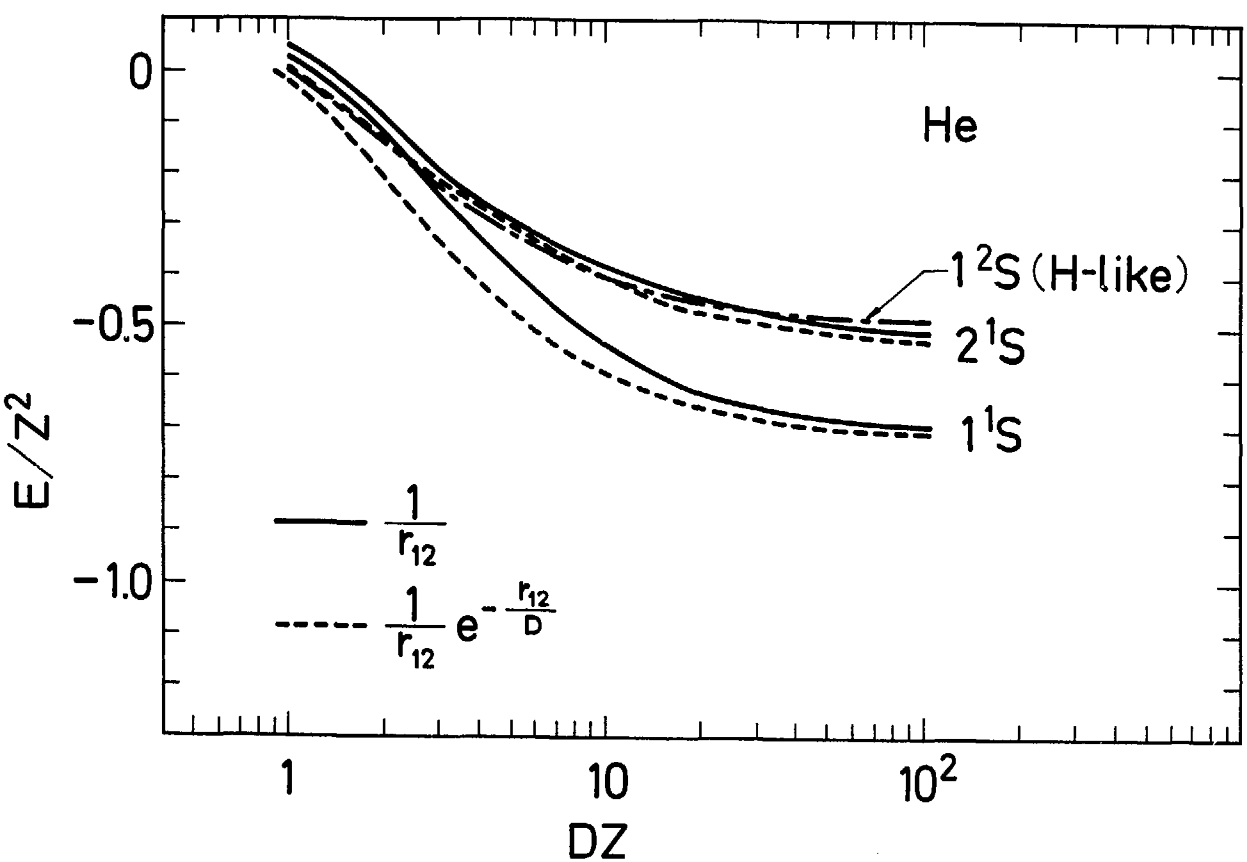
Figure captions

Fig.1 Dependences of the total energy levels on the screening lengths for the 1^1S and 2^1S state in He I, and for the 1^2S states in He II.
----- : 1^2S, Rogers et al.(Ref.6) ; ——— : the case of $D_{12}=\infty$; ----- : the case of $D_{12}=D$.
E/Z^2 and DZ are in atomic units.

Fig.2 Dependences of the total energy levels on the screening lengths for the 1^1S, 2^1S and 3^1S states in O VII, and for the 1^2S states in O VIII.
----- : 1^2S, Rogers et al. (Ref.6) ; ——— : the case of $D_{12}=\infty$; ----- : the case of $D_{12}=D$.

Fig.3 Dependences of the total energy levels on the screening lengths for the 1^1S, 2^1S and 3^1S states in Fe XXV, and for the 1^2S state in Fe XXVI. Explanations for curves are the same as in Fig.2.

Fig.4 Ion-coupling parameters on the Debye screening lengths for various electron densites and electron temperatures in Z=2 and Z=8. ——— : Z=2 and ----- : Z=8.



He
1^2S (H-like)
2^1S
1^1S
$\frac{1}{r_{12}}$
$\frac{1}{r_{12}} e^{-\frac{r_{12}}{D}}$
0
−0.5
−1.0
E/Z^2
1
10
10^2
DZ

Fig. 1

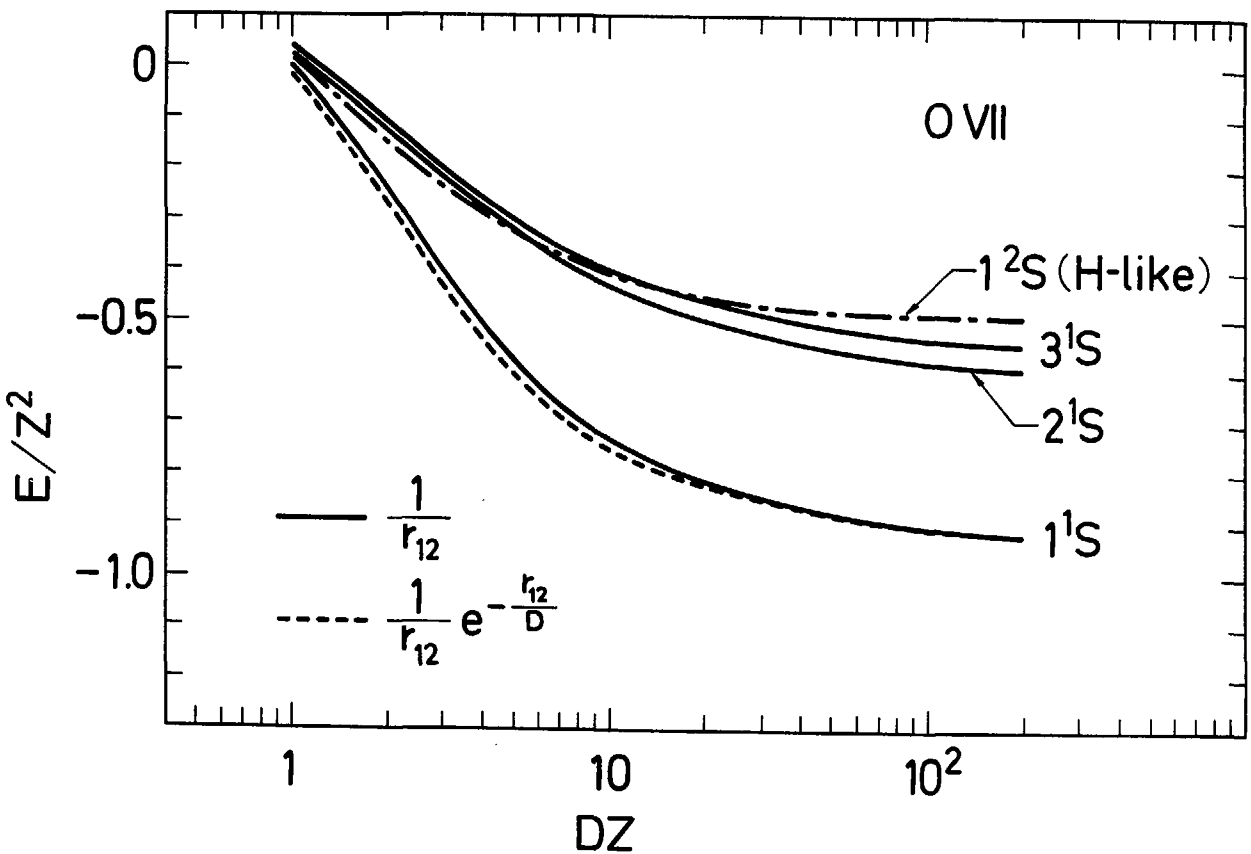

O VII
1 2S (H-like)
3 1S
2 1S
1 1S
1/r12
1/r12 e^-r12/D
E/Z2
0
-0.5
-1.0
1
10
10 2
DZ

Fig.2

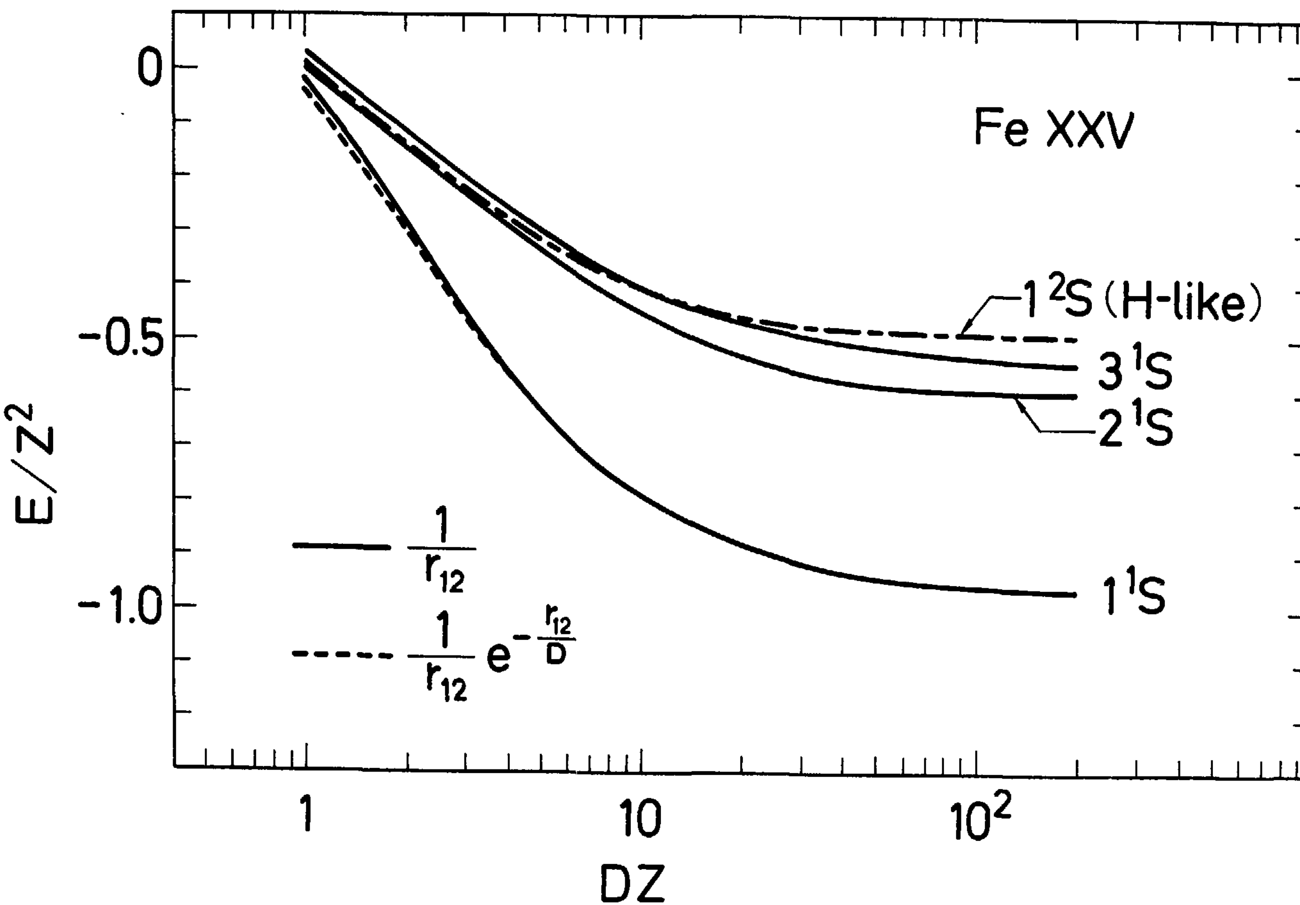
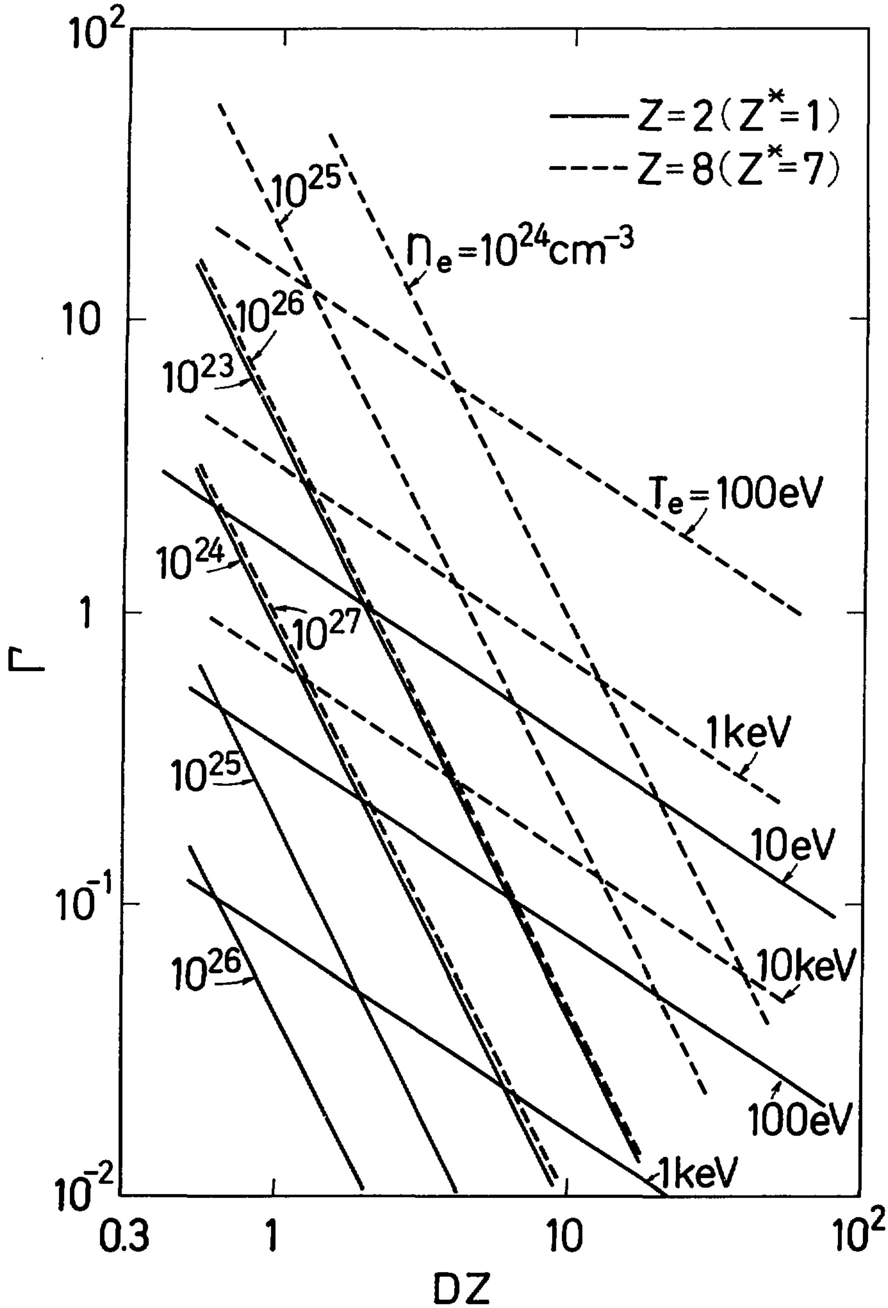

Fe XXV
$1\,^2S$ (H-like)
$3\,^1S$
$2\,^1S$
$1\,^1S$
$\frac{1}{r_{12}}$
$\frac{1}{r_{12}} e^{-\frac{r_{12}}{D}}$
0
-0.5
-1.0
E/Z^2
1
10
10^2
DZ

Fig.3

Fig.4



Z=2(Z*=1)
Z=8(Z*=7)
10^25
n_e=10^24 cm^-3
10^26
10^23
T_e=100eV
10^24
10^27
1keV
10^25
10eV
10keV
10^26
100eV
1keV
10^2
10
1
10^-1
10^-2
Γ
0.3
1
10
10^2
DZ