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# Statistical Description of Ionization Potentials in Dense Plasmas

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**Abstract.** The Thomas-Fermi model is used to investigate the influence of the density on the energies of ions in high-density plasmas ($\cong 10^{21}$–$10^{26}\,\mathrm{cm^{-3}}$). This model can be used to explain the two dominant high-density effects – continuum lowering and pressure ionization – by simple energy considerations. The result shows that only the outermost electrons are affected and that the inner region of the ion is hardly influenced by the density.

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Plasmas of densities in the range $\cong 10^{21}$–$10^{26}$ atoms/ions $\mathrm{cm^{-3}}$ exist by virtue of the irradiation of solids by short pulses and inertial confinement experiments, and are also expected in $Z$-pinch experiments [1–3]. In the case of such dense plasmas there is a strong interaction between the ions, i.e. the orbits of neighbouring atoms overlap and conducting bands occur. This lowers the binding energy of the electrons, and the energy gap between free and bound electrons decreases, which in turn leads to the lowering of the ionization potentials. If the density is high enough, this can lead to so-called pressure ionization.

Several authors [4–6] have used a statistical mechanics approach to investigate the effects of continuum lowering and pressure ionization. Because of the increasing complexity of this kind of description with higher $Z$ this method has only been used to investigate simple atoms like hydrogen, charge-symmetric plasmas or noble gases with high accuracy. In this paper the Thomas-Fermi (TF) model [7] is used to describe atoms in high-density matter. Although the TF model is less accurate than quantum mechanical descriptions using the Schrödinger equation, it enables one to investigate the influence of high density in complex high-$Z$ atoms with relatively little effort. Eliezer et al. [8] applied the TF model to calculate the density-dependence of the energy of the *atom* in dense matter. In this letter the model is generalized to describe *ions* at these densities. Only the simply TF model will be used and the corrections to it [9–11] will not be considered, because here the aim is more the qualitative understanding rather than quantitative investigations.

It will be shown up to which density the virial theorem of the free atom, $E_k = -\frac{1}{2} E_p$, is still valid. An explanation for the occurrence of pressure ionization will be given and it will be shown how the ionization potentials decrease. The result will demonstrate that the single ionization potential is almost unaffected up to a certain density, after which it drops to zero very quickly. After that the next highest ionization potential starts to decrease.

## Pressure Ionization and Continuum Lowering

The statistical model for atomic electrons was originally derived by Thomas [12] and Fermi [13] to investigate free many-electron atoms. Later on it was shown [7] that the model can be successfully used to describe high-density plasmas.

The statistical theory of the atom is based on the assumption that the electrons of the system can be treated as a degenerate electron gas in a self-consistent electrostatic field. The electron gas is described by Fermi-Dirac statistics, which in the case of full degeneracy,

$$n_i \geq 1.4 \times 10^{23}\,\frac{1}{Z}\left(\frac{kT}{10\,\mathrm{eV}}\right)^{3/2}, \qquad (1)$$

reduces to the Pauli principle. This means that for high enough densities the problem becomes temperature independent. In this case, if all effects other than the electrostatic interaction are neglected, the energies of the atoms

⋆ Present address: Heavy Ion Plasma Physics, Gesellschaft f. Schwerionenforschung, Planckstrasse 1, Postfach 110552, W-6100 Darmstadt, Fed. Rep. Germany and ions are given by: the kinetic energy $E_{\mathrm{kin}}$; the potential energy of the electron gas in the potential field of the core $E_{\mathrm{p}}^{\mathrm{v}}$; and the energy of the electrostatic interaction $E_{\mathrm{p}}^{\mathrm{int}}$. Thus

$$E = E_{\mathrm{kin}} + E_{\mathrm{p}}^{\mathrm{V}} + E_{\mathrm{p}}^{\mathrm{int}} \tag{2}$$

$$= C_1 \int n_{\mathrm{e}}^{5/3} d^3r - e \int V n_{\mathrm{e}} d^3r + \frac{e^2}{2} \iint \frac{n_{\mathrm{e}}(r) n_{\mathrm{e}}(r')}{|r-r'|} d^3r d^3r' . \tag{3}$$

with $C_1 = \frac{3}{10}(3\pi^2)^{2/3} e^2 a_0$ and $n_{\mathrm{e}}$ is the electron density. The variation $\delta(E - V_0 N_{\mathrm{e}}) = 0$, the Poisson equation and the substitutions $x = r/\mu$, $\mu = Z^{-1/3}(3\pi/4)^{2/3}\hbar^2/2me^2$ and $\Phi = r(V - V_0)/Ze$ give the Thomas-Fermi equation

$$\Phi'' = \frac{\Phi^{3/2}}{x^{1/2}} . \tag{4}$$

The boundary conditions for a neutral plasma are

$$\Phi(0) = 1; \quad \Phi(x_0) - x_0 \Phi'(x_0) = 0 , \tag{5}$$

where $x_0$ is the boundary of the elementary cell. In the case of high density matter the ion sphere radius is determined by the density $n_i = (4\pi r_0^3/3)^{-1}$ and the size of the elementary cell is given by $x_0 = r_0/\mu$.

The above-described plasma is neutral but consists of course of atoms and ions of different charge. To establish the influence of the density on a single ion of charge $Z-N$ in this neutral plasma the boundary condition is replaced by

$$\Phi(0) = 1; \quad \Phi(x_0) - x_0 \Phi'(x_0) = q \tag{6}$$

with $q = (Z - N)/Z$, where $N$ is the number of bound electrons.

The electron density is then given by

$$n_e(r) = \frac{Z}{4\pi\mu^3} \left( \frac{\Phi(x)}{x} \right)^{3/2} . \tag{7}$$

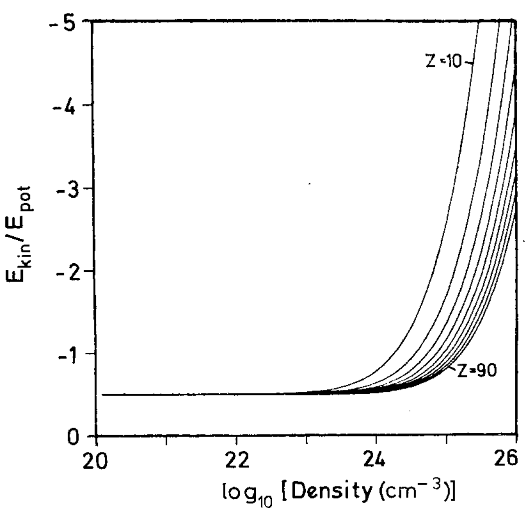


**Fig. 1.** Ratio of $E_{\mathrm{kin}}$ and $E_{\mathrm{pot}}$ for $Z = 10, 20, \ldots, 90$ as a function of the density

So the kinetic energy can be rewritten as

$$E_{\mathrm{kin}} = \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} \int n_{\mathrm{e}}^{5/3} d^3r = \frac{3}{5} \frac{e^2}{a_0} \frac{(2Z)^{7/3}}{(3\pi)^{2/3}} \int_0^{x_0} \frac{\Phi^{5/2}}{x^{1/2}} dx . \tag{8}$$

Solving the integral (see e.g. [8]) and using the boundary conditions, the kinetic energy of the ions is given by

$$E_{\mathrm{kin}} = \frac{3}{7} \frac{e^2}{a_0} \frac{(2Z)^{7/3}}{(3\pi)^{2/3}} \times \left( -\Phi'(0) + q \frac{\Phi_0}{x_0} - \frac{q^2}{x_0} + \frac{4}{5} x_0^{1/2} \Phi_0^{5/2} \right), \tag{9}$$

where $\Phi_0$ is the abbreviation for $\Phi(x_0)$. The potential energy of the electron gas in the potential field is

$$E_{\mathrm{p}}^{\mathrm{V}} = -e \int V_{\mathrm{F}} n_{\mathrm{e}} d^3r = -\frac{Z^2 e^2}{\mu} \int_0^{x_0} \frac{\Phi^{3/2}}{x^{1/2}} dx = -\frac{Z^2 e^2}{\mu} \left( \frac{\Phi_0 - q}{x_0} - \Phi'(0) \right). \tag{10}$$

The electrostatic interaction energy is given by

$$E_{\mathrm{p}}^{\mathrm{int}} = -e \int_0^{r_0} V_{\mathrm{int}} n_{\mathrm{e}}(r) d^3r$$

$$= -\frac{e}{2} \int_0^{r_0} n_{\mathrm{e}}(r) \left( V(r) - \frac{Ze}{r} \right) d^3r$$

$$= -\frac{Ze}{2} \left( \frac{Ze}{\mu} \int_0^{x_0} \frac{\Phi^{5/2}}{x^{1/2}} dx + V_0 \int_0^{x_0} x^{1/2} \Phi^{3/2} dx - \frac{Ze}{\mu} \int_0^{x_0} \frac{\Phi^{3/2}}{x^{1/2}} dx \right)$$

$$= -\frac{Z^2 e^2}{\mu} \left( \frac{1}{7} \Phi'(0) + \frac{2}{7} x_0^{1/2} \Phi_0^{5/2} + \frac{q}{x_0} (\Phi_0 - q) - \frac{\Phi_0 - q}{x_0} \right). \tag{11}$$

As shown in [8] the virial theorem can be written in the form $2E_{\mathrm{kin}} + E_{\mathrm{pot}} = 3PV$, where $P$ is the pressure and $V$ the volume. This of course should not depend on the density. For free atoms the virial theorem simplifies to $E_{\mathrm{kin}} = -\frac{1}{2} E_{\mathrm{pot}}$. Figure 1 shows that this free atom equation is valid up to densities of $10^{23}\,\mathrm{cm}^{-3}$. This is surprising in view of the strong interactions of the atoms at these densities. Summing (9–11) the energy of the ions

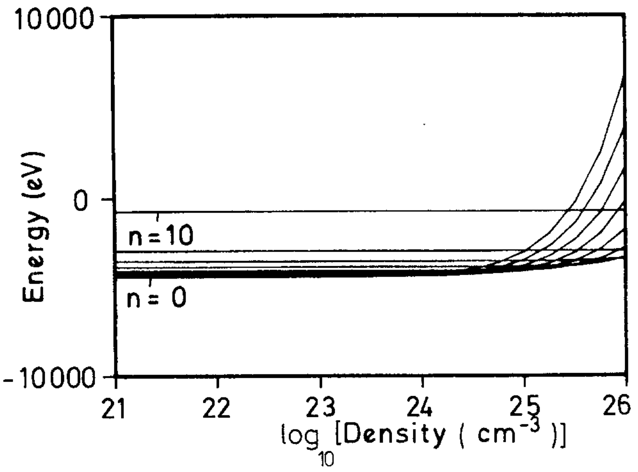


**Fig. 2.** Dependence of the total energy of the Ne atom and its ions on the density

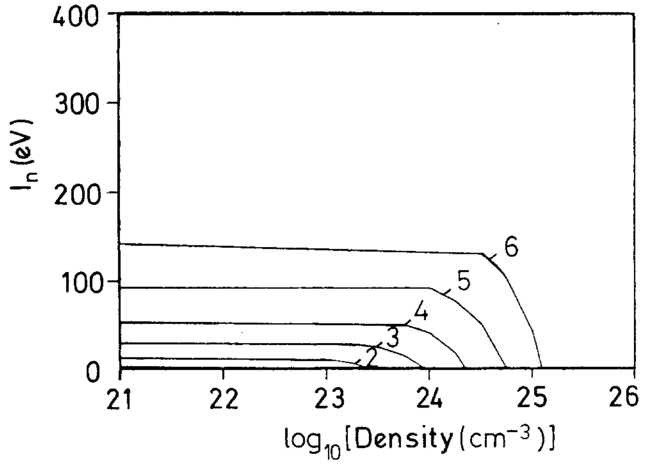


**Fig. 3.** Density dependence of the ionization potentials using the TF model

in a dense plasma is obtained as

$$E = -\frac{Z^2e^2}{\mu}\left(-\frac{3}{7}\Phi'(0) + \frac{2}{35}x_0^{1/2}\Phi_0^{5/2} + \frac{3}{7}\frac{q}{x_0}(\Phi_0 - q)\right). \tag{12}$$

Approximation formulae for $\Phi(x_0)$ are given by March [14]. The new result of (12) includes the well-known special case of the atom in a plasma [8] with $q = 0$

$$E_{\mathrm{AP}} = -\frac{Z^2e^2}{\mu}\left(-\frac{3}{7}\Phi'(0) + \frac{2}{35}x_0^{1/2}\Phi_0^{5/2}\right) \tag{13}$$

and the free atom [7] with $\Phi(x_0 = \infty) = 0$

$$E_0 = \frac{Z^2e^2}{\mu}\frac{3}{7}\Phi'(0) \tag{14}$$

with $\Phi'(0) = -1.588$.

Figure 2 shows the density-dependence of the energy of the Ne atom and its ions. It can be seen that at a certain density the energy of the atom is higher than that of the singly ionized atom. The ion is therefore more likely to exist than the atom at this density. This explains the effect of pressure ionization.

The energy $Q_n$ which is needed to transfer a neutral atom in a dense plasma into a special ionization state $n$ is given by

$$Q_n = E_n - E_{\mathrm{AP}} = \frac{Z^2e^2}{7\mu}\left\{3\left[\Phi_n'(0) - \Phi_{\mathrm{A}}'(0)\right] + \frac{2}{5}\left[x_{\mathrm{on}}^{1/2}\Phi_{\mathrm{on}}^{5/2} + (x_{\mathrm{0A}}^{1/2}\Phi_{\mathrm{0A}}^{5/2})\right] - 3\frac{n}{Zx_{\mathrm{on}}}\left(\Phi_{\mathrm{on}} - \frac{n}{Z}\right)\right\}, \tag{15}$$

where the index $n$ indicates an $n$-fold ionized state and A a neutral atom. The ionization energy is then simply obtained as

$$I_n = Q_n - Q_{n-1}. \tag{16}$$

Figure 3 shows the density dependence of the ionization potentials. The ionization potentials decrease with increasing density. But not all electrons of the atom are influenced in the same way. The single ionization potential is almost unchanged until it reaches a certain density, after which it decreases very rapidly. When the $n$th ionization potential reaches zero, the $(n+1)$th potential starts to decrease. So electrons leave the atom one after another.

## Conclusions

A simple formula for the energy of ions in dense plasmas has been derived by using the TF model. This simple expression allows one to describe the following effects:

- Figure 1 showed that the virial theorem of the free atom is valid up to surprisingly high densities of $10^{23}\,\mathrm{cm}^{-3}$.
- Pressure ionization: A comparison of these energies shows that at a special density the energy of the atom is higher than that of the ions. So in this instance the existence of ions is more probable than that of atoms, which explains the effect of pressure ionization.
- Continuum lowering. The lowering of the ionization potentials has been calculated within the TF model. The result was that the single ionization potential is almost unaffected until a certain density is reached, after which it drops to zero very quickly. After that the next highest ionization potential starts to decrease. The result shows only the outermost electrons get affected by density variations and that the inner region of the ion remains nearly uninfluenced by the density. This can be thought of as "density screening" of the nucleus.

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