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Nearest-neighbor effects in hot and dense plasmas: Thermodynamic properties

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A model for describing the influence of the nearest-neighbor interaction on the thermodynamic properties of plasmas is presented. This model is a generalization of the Thomas-Fermi model to cylindrical symmetry. The model was applied to the calculation of the electric potential of a pair of identical ions. An iron plasma at an ion density of 10^{23} cm^{-3} at a range of temperatures of practical interest was used to illustrate the predictions of the model. The ionization-potential reduction, the ion-pair free energy, and the average distance to the nearest neighbor were calculated. Our results indicate that the inclusion of the nearest-neighbor interaction predicts a plasma which is slightly more compressible than predicted by the spherically symmetric Thomas-Fermi model.

I. INTRODUCTION

The effort concentrated in recent years on the research into hot and dense plasmas, particularly astrophysical and laser-produced plasmas, has stimulated extensive theoretical investigation on the behavior of atoms in these plasmas and the influence of the plasma environment on atomic properties.[1–6] In particular, it was found that the screening of the nuclear potential by the free electrons shifts the energy levels, modifies the bound-electron wave functions, and changes the cross sections of the atomic processes with the plasma density.[7–10]

The models used to describe the behavior of ions in hot and dense plasmas generally assume a single-particle spherically symmetric ionic potential. The assumption of a spherically symmetric potential seems to be plausible for some temperature and density domains. It is equally plausible that at other domains of temperature and density the interaction between neighboring ions makes the spherical potential inadequate for the description of the atomic electrons. This particularly holds true when the plasma conditions are such that considering a certain ion, the probability of finding one of the neighboring ions significantly closer than the others is quite large. We expect these conditions to hold when the ion coupling parameter Γ is not very large. In that case, the average ionic field has an appreciable cylindrical component, which may affect the atomic and thermodynamic properties of the plasma. Also, for very small values of Γ the effect of this cylindrical component becomes negligible because of the low particle density in the regions where the cylindrical component is appreciable. For very high values of Γ a lattice-type structure builds up in the plasma, and the symmetry around each ion is of cubic type. This case is out of the scope of this paper. Therefore, the density and temperature domain in which the presence of the nearest neighbor can be important is restricted to intermediate values of Γ, somewhere between 0.1 and 10. The boundaries of this domain depend, however, on the specific plasma property under consideration.

It is the aim of this paper to study the distortion of the average ionic potential from a spherical to cylindrical symmetry, and to investigate the consequences of this distortion on the various thermodynamic properties of the plasma.

II. CYLINDRICAL THOMAS-FERMI MODEL

A. Basic assumptions

In our model we consider explicitly only the interaction of an ion with its nearest neighbor. The effect of the other ions is taken into account through a confined-molecule model which assumes zero potential outside the volume of the two ions, similar to the spherically symmetric models. The Born-Oppenheimer approximation is assumed to hold true, namely, that the electron cloud adjusts itself rapidly to the local electric field of the ions, i.e., the state of the electron cloud is determined uniquely by the instantaneous distance between the two ions. While the innermost electrons are perturbed only slightly by the neighboring ion, the highly excited states may be deformed so strongly that they overlap both ions, thereby generating a quasimolecule. Any slight perturbation moves such an electron farther away from this quasimolecule so that it should be better regarded as bound to the plasma as a whole rather than to any ion separately. Eventually, such an electron will collide with a free electron and will be absorbed into the thermal statistical free-electron distribution.

For simplicity, we used the Thomas-Fermi model to study the properties of such a quasimolecule and its influence on the plasma parameters. Other models, such as self-consistent-field or more realistic models, could be used as well.

One more assumption is incorporated in our model: it was shown[11] that for constant electron density the electric field of such a quasimolecule vanishes on the boundaries if these boundaries have a peanutlike shape. Moreover, for such a peanut-shaped molecule the potential energy of a quasimolecule is minimum for variations of the boundaries which keep the volume constant.[11] A similar shape is expected for more realistic electron distributions, such as those obtained from the Thomas-Fermi model. In the present model the shape of this molecular volume is approximated by two adjacent truncated spheres (see Fig. 1), each having volume τ. It turns out that when the requirements of charge neutrality and zero potential on the boundaries of such a volume are imposed, the electric field on the outer surface is small (compared to the average plasma microfield), except on the circle connecting the two spheres; see Fig. 2. Therefore, although the electric field does not completely vanish outside the molecular volume, such quasimolecules can be regarded as electrically isolated to a high degree of accuracy. This point is further discussed in Sec. III.

The volume of one of the truncated spheres is

$$\tau=\pi(\tfrac{2}{3}R_s^3+\tfrac{1}{2}R_s^2R-\tfrac{1}{24}R^3)\ , \tag{1}$$

where R_s is the radius of the spherical portion and R is the distance between the centers of the two spheres.

Contrary to the spherically symmetric case, the volume of the quasimolecule, 2τ, is not uniquely determined by the average density of the plasma. In our case, the volume τ for a given Fermi energy depends on the interionic distance R, as can be seen from the following extreme cases: (i) when $R=2R_s$, we have two spheres each having the same volume, denoted by τ_1; (ii) when $R=0$ the two spheres merge to a single spherical ion having nuclear charge $2Z$ and volume denoted by $2\tau_2$.

Spherically symmetric Thomas-Fermi calculations show that for the same temperature and quasimolecular volume (i.e., $\tau_2=\tau_1$), the Fermi energy of case (i) is higher than that of case (ii). Therefore, to obtain equal Fermi energies for the two cases, τ_2 should differ from τ_1. Since the Fermi energy is constant in the plasma, this means that the volume τ of a particular quasimolecule depends on the interionic distance R. The method used here to determine the function $\tau(R)$ is described in Sec. III. The average quasimolecular volume is $2\tau_0$, where

$$\tau_0=\frac{1}{n_i}=\frac{4\pi}{3}R_i^3\ . \tag{2}$$

Here n_i is the ion density and R_i is the ion sphere radius.

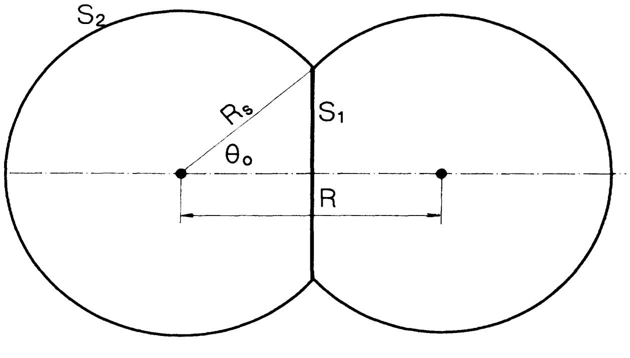

FIG. 1. Approximate shape of the quasimolecule.

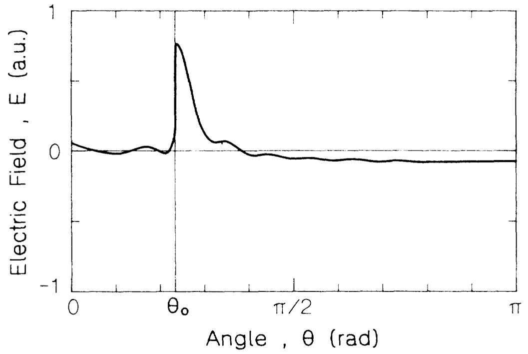

FIG. 2. Normal component of the electric field on the boundary of the truncated sphere, for iron plasma at a density of 10^{23} cm^{-3}, temperature of 300 eV, and interionic distance $R=3.80$ a.u. Points on the interionic boundary S_1 correspond to $0\leq\theta<\theta_0$ and points on the outer boundary S_2 correspond to $\theta_0<\theta\leq\pi$.

B. Mathematical procedure

Our starting point is the basic three-dimensional Thomas-Fermi equation, for a given quasimolecule of volume 2τ and interionic distance R,

$$\Delta V(\mathbf{r})=4\pi e C_{\mathrm{TF}} I_{1/2}\left[\frac{\varepsilon_F+eV(\mathbf{r})}{kT}\right]\ , \tag{3}$$

where ε_F is the Fermi energy,

$$I_j(x)=\int_0^\infty \frac{y^j dy}{e^{y-x}+1} \tag{4}$$

is the Fermi-Dirac integral of order j, and

$$C_{\mathrm{TF}}=\frac{1}{2\pi^2}\left[\frac{2mkT}{\hbar^2}\right]^{3/2}\ . \tag{5}$$

As the potential is symmetric with respect to a reflection through the interface S_1 between the two spheres (see Fig. 1), we may confine ourselves to the solution of Eq. (3) in a single truncated sphere. The potential $V(\mathbf{r})$ has to satisfy three boundary conditions.

(i) Near the nucleus,

$$\lim_{r\to 0} rV(\mathbf{r})=Ze\ , \tag{6}$$

where Z is the nuclear charge.

(ii) On the surface S_1 the normal electric field, i.e., the normal derivative of the potential should vanish,

$$\left.\frac{\partial V(\mathbf{r})}{\partial n}\right|_{S_1}=\left.\frac{\partial V(\mathbf{r})}{\partial z}\right|_{z=R/2}=0\ , \tag{7}$$

where z is the coordinate along the symmetry axis.

(iii) One would like that the electric field would vanish also on the spherical portion, S_2, of the truncated sphere. This condition means that there is no electric field outside the volume of the quasimolecule so it is electrically isolated and the electronic free energy is at a minimum with respect to shape variations.[12] This condition, however, cannot be satisfied rigorously, because the shape of the molecule is already determined. Instead, two weaker conditions are imposed: (a) the molecule is electrically neutral, and (b) the boundary of the molecule is the equipotential surface of $V=0$,

$$\int_{S_2} \frac{\partial V}{\partial n} dS = 0 , \tag{8a}$$

$$V(\mathbf{r}\varepsilon S_2) = 0 . \tag{8b}$$

Equation (3) with the boundary conditions (6), (7), (8a), and (8b) has a unique solution. If our choice of the shape of the molecular boundaries is sufficiently close to the accurate ones, the electric field on the boundary S_2 is expected to be small.

To solve Eq. (3) with the above boundary conditions the potential is expanded into its multipole components,

$$V(\mathbf{r}) = V_0(r) + \sum_{k=0}^{\infty} v_k(r) P_k(\mu) . \tag{9}$$

Here $V_0(r)$ is chosen to be the spherically symmetric Thomas-Fermi potential for ionic volume τ_0 and nuclear charge Z, and $P_k(\mu)$ are the Legendre polynomials of the argument $\mu = \cos\theta$.

The sum in Eq. (9) represents the cylindrical component of the potential. In the following we assume that for the phenomena investigated in this paper, the influence of the cylindrical distortion, as well as the change in the Fermi energy $\varepsilon_F - \varepsilon_F^0$ caused by the formation of quasimolecules in the plasma, are small relative to the spherically symmetric solutions and can be treated in first-order perturbation theory. Substituting Eq. (9) in Eq. (3) and using the first-order expansion of the Fermi-Dirac integral,

$$I_{1/2}(x_0+\delta) \approx I_{1/2}(x_0) + \frac{\delta}{2} I_{-1/2}(x_0) , \tag{10}$$

the following second-order differential equation is obtained for the multipole coefficients:

$$v_k'' + \frac{2}{r} v_k' - \frac{k(k+1)}{r^2} v_k = \frac{2\pi e^2}{kT} C_{\mathrm{TF}} I_{-1/2} \left[\frac{\varepsilon_F^0 + eV_0(r)}{kT} \right] (v_k + \eta \delta_{k,0}) , \tag{11}$$

where

$$\eta = (\varepsilon_F - \varepsilon_F^0)/e . \tag{12}$$

The boundary condition, Eq. (6), implies

$$\lim_{r \to 0} r v_k(r) = 0 . \tag{13}$$

The other boundary conditions, Eqs. (7) and (8), couple the various v_k's and thus determine the particular solution of the homogeneous part of Eq. (11). In practice, only a finite number of terms (generally $k_{\max} \le 30$) were taken into account in the expansion Eq. (9), and the boundary conditions can be satisfied only in a least-squares sense. The details of such a least-squares procedure are explained in the Appendix.

III. RESULTS AND DISCUSSION

Figure 3 shows equipotential lines of an iron quasimolecule in a plasma of ion density 10^{23} cm^{-3} and temperature 300 eV. The interionic distance is $R = 1.5R_i$ ($R_i \sim 2.53$ a.u.), and 30 multipole terms are used in the expansion of the potential. It can be seen that near the nuclei the equipotential lines are almost circular, which means that the deeply lying ionic states are almost unaffected by the formation of the quasimolecule. On the other hand, near the outer boundary of the quasimolecule the equipotential lines surround both nuclei and thus the higher electronic states of the ions are significantly altered and become molecular states.

The transition from discrete ionic to quasimolecular states occurs when the energy of the bound electron approaches the energy associated with the saddle point of the potential positioned halfway between the two ions. The lowest quasimolecular states are bound to, at least, a pair of ions. For the higher states the spatial range of the electronic wave function increases with the energy, and overlaps more and more ions, thus creating a smooth transition from quasimolecular to continuum states. Figure 4 shows the saddle-point energy at a constant density of $n_i = 10^{23}$ cm^{-3} and a range of temperatures when the two ions are separated by the average interionic distance (see below) corresponding to the given plasma conditions.

The ionization energy reduction in the quasimolecule is somewhat smaller than the one predicted by the spherical model,[6,13] and depends strongly on the temperature and interionic distance. This deviation can be approximated by $(\bar{Z}/Z)v_0(0)|_{T=\infty}$ ($\bar{Z}$ is the average ionic charge) for a given interionic distance R. For the average interionic distance this deviation is less than 22% of the value predicted by the spherical model. The ionization energy reduction is shown in Fig. 4 both for the quasimolecular model and the ion sphere model.

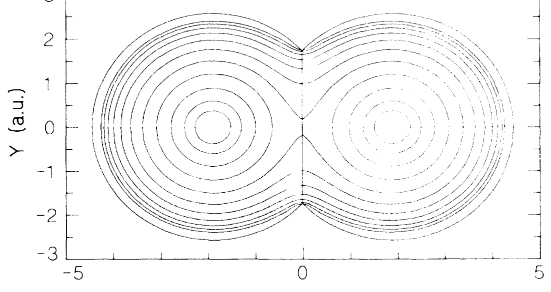

FIG. 3. Equipotential contours in the quasimolecule of Fig. 2. The central circle around the nucleus corresponds to electron potential of 1 keV. The potential energy is changed by a factor of 2 between two adjacent contours.

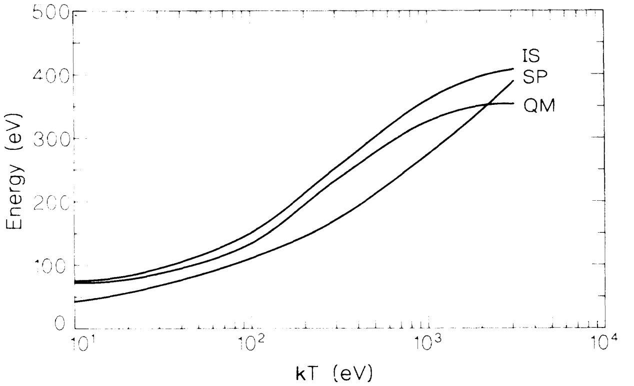

FIG. 4. Ionization energy reduction as a function of the temperature in the present paper (QM) and in the ion-sphere model (IS). The ion separation equals the average interionic distance (see Fig. 9). Also shown is the absolute value of the potential energy of an electron located at the saddle point (SP).

The electric field outside the quasimolecule is not exactly zero (as can be seen from Fig. 2), and therefore the quasimolecule is not completely isolated electrically. Increasing the number of the multipole terms in Eq. (9) will reduce the normal electric field on the interface S_1 between the two ions. We do not expect, however, that the electric field on S_2 will vanish as $k \rightarrow \infty$. The reason for this is the deviation of the shape of the boundary of the quasimolecule from the ideal shape which would ensure zero field outside the boundary, and we assume that only the average field vanishes on S_2, Eq. (8a). The root mean square of the electric field on the boundary S_2 is defined by

$$\overline{\Delta E}=\left[\frac{1}{S_2}\int_{S_2}E^2dS\right]^{1/2} . \qquad (14)$$

The quantity $e\overline{\Delta E}R_s/kT$ is a measure of the energy associated with the nonvanishing electric field outside the quasimolecule compared to the thermal energy of a free electron. This quantity is shown in Fig. 5, which shows that this quantity is relatively small, thereby confirming the basic assumptions of our model. It also shows that the higher the temperature and the farther the separation between the ions, the smaller the inaccuracies in the free energy due to neglect of the electric field outside the quasimolecule.

Figure 6 shows the Fermi energy at constant quasimolecule volume as a function of the interionic distance R for the same plasma conditions as in Fig. 3. The two extreme points, $R=0$ and $R=2R_i$, were calculated with the spherically symmetric Thomas-Fermi model. The Fermi energy is seen to be a monotonically increasing function of the interionic distance. Our calculations show that this feature holds true for a wide range of temperatures and densities.

Figure 7 shows the ratio $\tau(R)/\tau(2R_i)$ at constant Fermi energy as a function of the interionic distance R. As we shall see later, the average interionic distance is considerably smaller than $2R_i$ ($\sim R_i$ for the above ion plas-

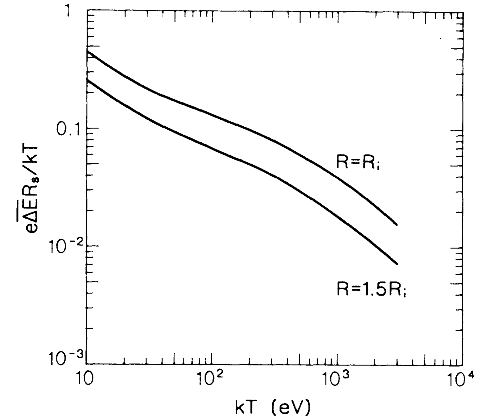

FIG. 5. Average normal electric field, $\overline{\Delta E}$ in units of kT/eR_s, on the outer boundary S_2 of the quasimolecule as a function of the temperature for two interionic distances. The plasma conditions are the same as in Fig. 2 and R_i is the ion sphere radius.

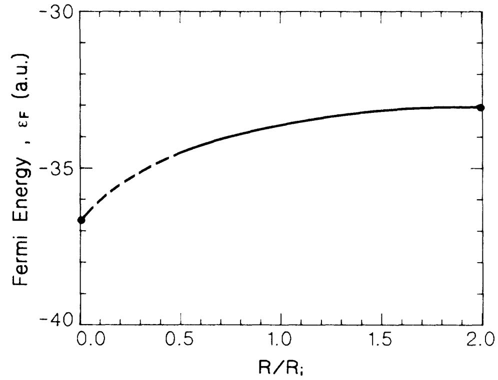

FIG. 6. Fermi energy ε_F of an iron plasma at $T=300$ eV, as a function of the interionic distance, for constant volume $2\tau_0$ of the quasimolecule. The two extreme points were calculated by the spherically symmetric Thomas-Fermi model. The dashed portion of the line is a free-hand interpolation.

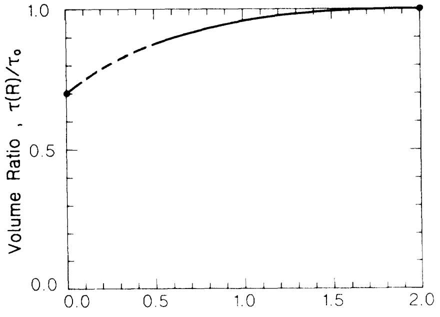

FIG. 7. Volume $\tau(R)$ of the truncated sphere of an iron plasma at $T=300$ eV as a function of the interionic distance for constant Fermi energy. The Fermi energy is the value obtained for a plasma density of 10^{23} cm^{-3} in a spherically symmetric Thomas-Fermi model.

ma conditions). It follows that the present model predicts a plasma which is more compressible than predicted by the spherical TF model. Figure 7 illustrates our conjecture, mentioned in Sec. II, that for constant Fermi energy and plasma temperature, the volume of the quasimolecule varies with the interionic distance. One should note that this volume exhibits a monotonic smooth behavior which enables an easy interpolation toward $R \to 0$, which is again a spherically symmetric case.

Figure 8 shows the Gibbs free energy F of the quasimolecule at rest at constant pressure P, as a function of the interionic distance. This function, which is the central result of this paper, is the basis from which the thermodynamic properties were derived. The free energy is computed from its definition,

$$F=E+PV-TS \;, \tag{15}$$

where E is the internal energy incorporating the electron-electron, electron-ion, and ion-ion potential energies and the electron kinetic energy,

$$E=E_p^{e\text{-}e}+E_p^{e\text{-}i}+E_p^{i\text{-}i}+E_k^{e} \;, \tag{16}$$

$V=2\tau$ is the volume of the quasimolecule, and S is the entropy. The various quantities were calculated using the standard TF expressions taking into account the shape of the quasimolecule.

The average nearest-neighbor distance $\bar{R}$ was calculated by the Monte Carlo method using the quasimolecule free energy $F(R)$ as an interionic potential. Let D denote a random instantaneous spatial distribution of the ions in the plasma, then,

$$\bar{R}=\frac{\sum_{D} W^{(D)} R_{\min}^{(D)}}{\sum_{D} W^{(D)}} \;, \tag{17}$$

where $R_{\min}^{(D)}$ is the distance between a given ion (located at the origin) and its nearest neighbor in the distribution D, and $W^{(D)}$ is a weight function given by

$$W^{(D)}=\exp\left[-\sum_{\text{pairs in } D} F(R_{\text{pair}})/kT\right] . \tag{18}$$

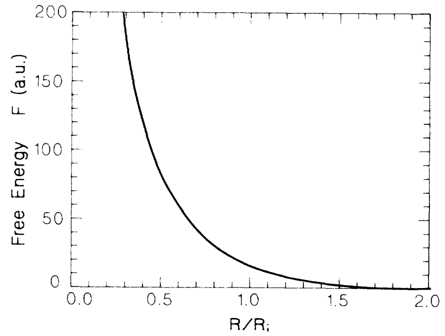

FIG. 8. Free energy of a quasimolecule as a function of the interionic distance for plasma conditions and Fermi energy as in Fig. 7.

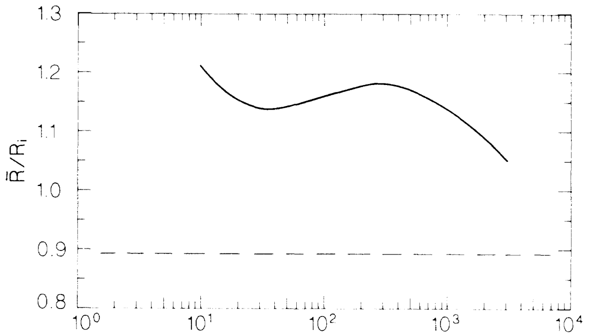

FIG. 9. Average nearest-neighbor distance as a function of the temperature for ion plasma at density equal to 10^{23} cm^{-3}. The dashed line corresponds to the average interionic distance of an ideal gas.

Figure 9 shows the average nearest-neighbor distance $\bar{R}$ as a function of temperature for an iron plasma at density of $n=10^{23}$ cm^{-3}. It can be seen that $\bar{R}(T)$ does not decrease monotonically as the temperature is increased. In fact, there is a local minimum around $T\approx 200$ eV. This structure arises from a competition between two effects: (i) as the temperature increases, so does the ionic kinetic energy, thus increasing the probability of interionic penetration; (ii) on the other hand, increasing the temperature increases the ionization, thereby reducing the screening of the nuclear charge and increasing the repulsive potential. At the two extremes of very low and very high temperatures the average interionic distance $\bar{R}(T)$ is a monotonically decreasing function. As the temperature approaches zero, the probability for the two ions to be closer than $2R_i$ becomes smaller, as can be seen from Fig. 8. At $T=0$ we get the ion-sphere distance $\bar{R}=2R_i$. However, at very low temperatures one would expect our model to break down as a cubic symmetry will build up in the plasma.

At very high temperatures the ions behave like uncorrelated ideal gas, and in this case,

$$\bar{R}(T)\to\tfrac{1}{3}\Gamma(\tfrac{1}{3})R_i\approx 0.893R_i \;. \tag{19}$$

A model for nearest-neighbor interactions in plasmas within the framework of the Thomas-Fermi approximation was recently developed by Laughlin.[14] In his model he assumes a spherical cell for the electric charge of each ion and the variation of the interionic distance is simulated by the displacement of the nucleus from the center of the sphere. The main differences between his model and the present one is the shape of the boundary of the ionic cell and the boundary conditions of the potential. For purposes of comparison, we repeated our calculation for an aluminum plasma of ionic radius of 4 a.u., which is the case study of Ref. 14, and found differences between the results of the two models. The main differences are the following. (i) The pressure in our model increases monotonically with the interionic distance, while the results in Ref. 14 show opposite tendency. This difference can be accounted for by the large contribution to the pressure in Ref. 14 from the interface between the two ions. In our

TABLE I. Changes of the electronic free energy of Al ions in plasma of ionic radius $R_i=4$ a.u. and temperature equal to 1 a.u. for various interionic distances.

R/R_i	Present paper	Ref. 14
1.875	0.01	0.015
1.75	0.024	0.06
1.68	0.033	0.10

work this interface is an internal part of the quasi-molecule and does not contribute to the pressure. (ii) The Fermi energy in Ref. 14 is not monotonic with respect to the temperature and the interionic distance, while our results show a monotonic behavior. (iii) The electronic free energy of the ions, relative to the case of separate ions, is significantly higher in Ref. 14 than in the present paper; see Table I. Since both papers solve the Thomas-Fermi equation, the model which gives the lower free energy for the same volume and temperature seems to be more reliable.

ACKNOWLEDGMENTS

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APPENDIX

In this appendix we describe the procedure to solve Eq. (11) with the boundary conditions given by Eqs. (6), (7), (8a), and (8b). If we denote

$$F(r)=\frac{e^2}{\pi kT}\left[\frac{2mkT}{\hbar^2}\right]^{3/2} I_{-1/2}\left[\frac{\varepsilon_F^0+eV_0(r)}{kT}\right] , \tag{A1}$$

then Eq. (11) can be rewritten as

$$v_k''+\frac{2}{r}v_k'-\frac{k(k+1)}{r^2}v_k=F(r)(v_k+\eta\delta_{k,0}) . \tag{A2}$$

For $k>0$, Eq. (A2) is homogeneous, therefore its solutions, which are regular at the origin, are determined up to a multiplicative factor β_k,

$$v_k(r)=\beta_k u_k(r) , \tag{A3}$$

where $u_k(r)$ is a particular solution of Eq. (A2).

For $k=0$ the general solution of Eq. (A2) is given by

$$v_0(r)=\beta_0 u_0(r)+\eta\omega(r) , \tag{A4}$$

where $u_0(r)$ is a particular regular solution of the homogeneous part of Eq. (A2), β_0 is a constant, and $\omega(r)$ is a particular solution of the inhomogeneous equation (A2),

$$\omega(r)=u_0(r)\int_0^r \frac{\int_0^y x^2 u_0(x)F(x)dx}{[yu_0(y)]^2}dy . \tag{A5}$$

The total potential now becomes

$$V(\mathbf{r})=V_0(r)+\eta\omega(r)+\sum_{k=0}^{\infty}\beta_k u_k(r)P_k(\mu) . \tag{A6}$$

The coefficients β_k and η are computed from the boundary conditions. This is carried out in two steps.

(i) Substituting $V(\mathbf{r})$ in Eq. (7), one gets

$$A(\mu)+\eta\omega'(r^*)\mu+\sum_{k=0}^{\infty}\beta_k B_k(\mu)=0 \quad \text{for } \mu_0\le\mu\le 1 , \tag{A7}$$

where

$$\mu_0=R/2R_s, \quad r^*=R/2\mu \tag{A8}$$

$$A(\mu)=V_0'(r^*)\mu , \tag{A9}$$

$$B_k(\mu)=u_k'(r^*)\mu P_k(\mu)+\frac{u_k(r^*)}{r^*}(1-\mu^2)P_k'(\mu) . \tag{A10}$$

(ii) From Eq. (8b) we get

$$C+\eta\omega(R_s)+\sum_{k=0}^{\infty}\beta_k D_k(\mu)=0 \quad \text{for } -1\le\mu\le\mu_0 , \tag{A11}$$

where

$$C=V_0(R_s) , \tag{A12}$$

$$D_k(\mu)=u_k(R_s)P_k(\mu) . \tag{A13}$$

The coefficients β_k and η are obtained by truncating the expansion of $V(\mathbf{r})$ in Eq. (9) at some multipole $k_{\max}$. Equations (A7) and (A11) are replaced by a least-squares minimalization procedure of the function $Q(\beta_0,\ldots,\beta_{k_{\max}};\eta)$ given by

$$\begin{aligned} Q&=\int_{S_1}\left[A(\mu)+\eta\omega'(r^*)\mu+\sum_{k=0}^{k_{\max}}\beta_k B_k(\mu)\right]^2 dS \\ &\quad +W\mu_0^2\int_{S_2}\left[C+\eta\omega(R_s)+\sum_{k=0}^{k_{\max}}\beta_k D_k(\mu)\right]^2 dS \\ &=\frac{\pi R^2}{2}\left[\int_{\mu_0}^{1}\left[A(\mu)+\eta\omega'(r^*)\mu+\sum_{k=0}^{k_{\max}}\beta_k B_k(\mu)\right]^2\frac{d\mu}{\mu^3}\right. \\ &\quad \left. +W\int_{-1}^{\mu_0}\left[C+\eta\omega(R_s)+\sum_{k=0}^{k_{\max}}\beta_k D_k(\mu)\right]^2 d\mu\right] . \end{aligned} \tag{A14}$$

Here W is an arbitrary weight function chosen so that the two sums in Eq. (A14) have the same dimensions,

$$W=\frac{\int_{S_1}(\partial V_0/\partial z)^2 dS}{\int_{S_1} V_0^2 dS}=\frac{\int_{\mu_0}^{1} A^2(\mu)d\mu/\mu^3}{\int_{\mu_0}^{1} V_0^2(R/2\mu)d\mu/\mu^3} . \tag{A15}$$

The final equations for the computation of the β coefficients are

$$\frac{\partial Q}{\partial \beta_k}=0 \quad \text{for } k=0,\ldots,k_{\max} . \tag{A16}$$

Substituting $V(\mathbf{r})$ in Eq. (8a) and truncating the sum at $k_{\max}$ gives

$$\int_{-1}^{\mu_0}\left[V_0'(R_s)+\eta\omega'(R_s)+\sum_{k=0}^{k_{\max}}\beta_k u_k'(R_s)P_k(\mu)\right]d\mu=0 . \tag{A17}$$

Equations (A16) and (A17) constitute $k_{\max}+2$ linear equations with $k_{\max}+2$ unknowns. The solutions β_k and η are inserted into Eqs. (A3) and (A4) to obtain the expansion of $V(\mathbf{r})$ and the change η in the Fermi energy caused by the nearest-neighbor interaction in the plasma.

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