Average-atom quantum-statistical cell model for hot plasma in local thermodynamic equilibrium over a wide range of densities

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(Received 17 July 1989)

A method for numerically modeling hot plasma over a wide range of densities is described. The model generalizes the essential aspects of the Stewart-Pyatt model to plasmas comprising mixtures of elements and extends the treatment to include the effects of electron polarization and screening. A practical numerical prescription is provided that is a straightforward generalization of the ion-sphere cell model. In addition, exact closed-form expressions are given for the continuum lowering. The model also addresses the problem of the microfield, i.e., the plasma-potential fluctuations that perturb the upper electronic states, and provides a suitable framework for improved practical approaches to this.

I. INTRODUCTION

Self-consistent-field average-atom models of hot local thermodynamic equilibrium (LTE) plasma generally fall into two generic groups: The spherical ion-cell (SIC) model—also called the ion-sphere model—considers the atomic ions in the plasmas to be centered inside neutral spheres which otherwise contain only electrons. This model is appropriate at high densities and/or low temperatures when the ions are sufficiently constrained by their mutual Coulomb repulsion for the ion cells to be *weakly overlapping* (Fig. 1). An example of an SIC model is the Wigner-Seitz model[1,2] used in the treatment of liquid metals. SIC models are commonly employed for calculating the opacities of laboratory-produced medium- to high-Z plasmas, and some high-density astrophysical plasmas.[3–8]

At very much lower densities the *average* potential at a reasonable distance from an ion is believed to resemble a Debye-Hückel screened potential which attains vanishing slope at infinity. The plasma is thus weakly polarized out to arbitrarily large distances and, since the potential does not (necessarily) have vanishing slope at the surface of the ion sphere, neutrality of the ion sphere cannot be guaranteed in accordance with the premises of the SIC model. This is because there is an appreciable probability of finding other ions inside the ion sphere of one particular ion. Neighboring ion spheres can overlap significantly. This situation occurs when the ions are able to move freely throughout most of the plasma (Fig. 2). Note that the potential in this model exists only by virtue of correlations with the central ion (which is afforded a special significance in the theory). I shall refer to models of this generic type (e.g., Refs. 9 and 10) as polarized correlation sphere (PCS) models. As high-temperature hydrogen plasmas are typically weakly coupled, this type of model is often preferred in astrophysical contexts.[11–13]

The apparent incompatibility of these two models presents an immediate problem when considering plasmas of intermediate coupling. Indeed, it turns out that medium-Z *Lorentzian* plasmas are typically in this regime and that the very high coupling strengths required to justify the SIC model are really those characteristic of liquid metals. This is the principal problem addressed by this paper.

The average-atom model[3–7] acquires its justification in the context of the canonical or grand canonical ensembles.[14] Here the plasma is considered as an ensemble of neutral atoms, each comprising an ion and a requisite number of unbound electrons. An approximated average over this ensemble yields the average atom. Thermodynamic properties of the plasma that relate to ensemble averages can then be deduced from the properties of the average-atom model with a reasonable degree of rigor. The picture seems to break down in the case of the PCS model which encompasses, not a single atom, but rather the whole plasma. Of course we could consider an ensemble of plasmas. The problem here is that the PCS

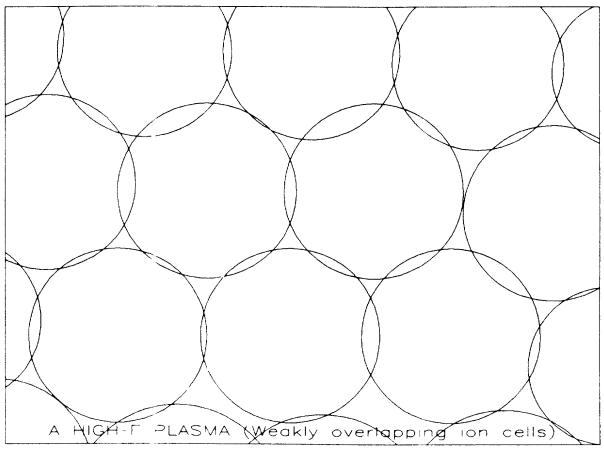

FIG. 1. Two-dimensional schematic representation of a high-Γ (high-density low-temperature) plasma, illustrating weakly overlapping ion spheres.

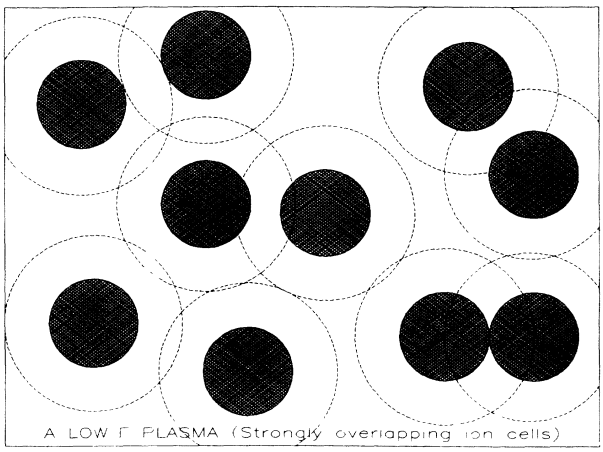

FIG. 2. Two-dimensional schematic representation of a lower (than in Fig. 1) Γ plasma illustrating strongly overlapping ion spheres. The shaded regions depict the ion cores which may be thought of as Landau spheres and which indicate the closest distances within which ions may typically approach each other.

model does not properly treat the plasma as a whole. Only the central ion is treated with the required degree of correctness. Thus there is evidently an ambiguity with regard to the extent of the thermodynamic system addressed by the model, a conceptual difficulty which is only overcome for the case of an isolated impurity ion immersed in a background plasma.

Another difficulty with the PCS model is that it often allows stable electron orbitals in regions where the existence of such orbitals is unlikely or impossible. (An artificial, often *ad hoc*, continuum lowering needs to be introduced to "remove" such states.) At large distances from the central ion, the PCS potential represents an average of a potential whose fluctuations are dominant in determining the behavior of an electron.

Both models have problems with arbitrarily composed mixtures (of different ion species, i.e., different elements) which is perhaps the clearest indication of their inadequacy. The SIC model works quite well provided *all* the components are strongly coupled to each other. The PCS model can accommodate impurities only at concentrations of less than one ion per Debye sphere.

A new *generalized ion-cell* (GIC) model, which extends some earlier ideas of Stewart and Pyatt, is proposed. This model overcomes all of the difficulties mentioned, if not directly, then by providing a theoretical framework that is sufficiently flexible to allow a treatment which does. The GIC model accommodates both SIC and PCS limits and interpolates continuously between them.

II. GENERALIZED ION-CELL MODEL

A. Notation and general remarks

Throughout the following ρ is used to denote electric charge density in units of the electronic charge e (>0), while V denotes the electrostatic potential. Therefore, in the absence of positive charges, the electron density will be $-\rho$ while the electronic potential will be $-V$.

The formulation applies to a *mixture* of average-atom ion species (i.e., different elements). The various mixture components are denoted by the subscript i. Thus n_i is the average (number) density of ions with atomic number Z_i in the plasma.

Only the electrostatic potential is considered here. Additional exchange and correlation components need to be taken into account when performing the quantum-mechanical part of the self-consistent-field calculation. However, once the self-consistent electrostatic potential is known, the other potential components are uniquely determined and therefore do not require an explicit or separate treatment. This is most evident in the general context of the local-density-functional approach,[15–26] which is almost universally adopted in average-atom computations.

B. Basis of the model

An underlying idea in the new model is the concept of a nonspherical ion cell as depicted in Figs. 3 and 4. It comprises an external region (of unspecified shape) containing *only* electrons surrounding a spherical core of radius r_i centered on an ion. The spatial average of the charge density in the external region is denoted by ρ_0. When treating the average atom, ρ_0 becomes the ensemble average of this quantity, which is the same as the average taken over the whole plasma. It is perhaps useful to point out at this stage that the nonspherical shape of the "typical ion" represented by Fig. 4 has no particular consequences in the theory that follows; i.e., no attempt is made to calculate any nonspherical terms in the potential. A principal reason for defining the ion cell in this way is to permit, at the outset, the exclusion of neighboring ions from the cell, which is not generally possible if the cell is defined to be spherical. This picture (Fig. 3) represents an instantaneous configuration of the ions in a

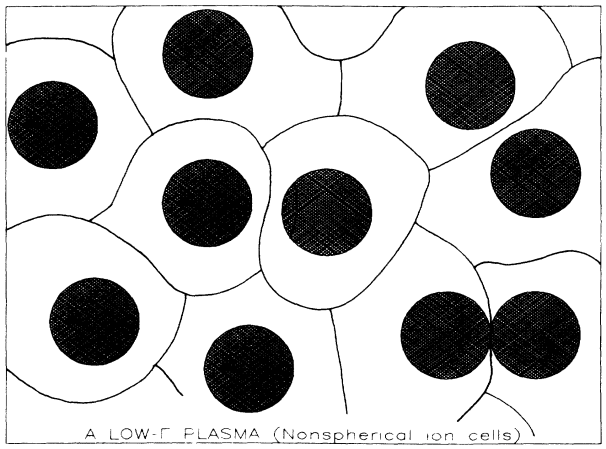

FIG. 3. Two-dimensional schematic represenation of the plasma depicted in Fig. 2 illustrating division of the plasma into nonspherical ion cells. These cells are electrically neutral regions each enclosing a single ion. Together, the cells fill the whole plasma without overlapping.

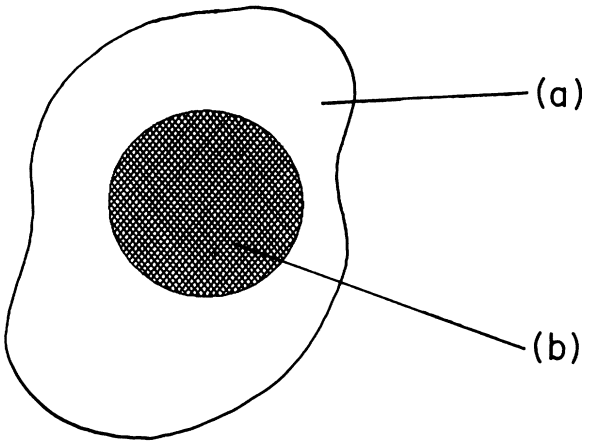

FIG. 4. The "fried egg" model. Components of a single nonspherical ion cell. (a) "external" plasma region (of unspecified arbitrary shape) containing only electrons at an average density of $-\rho_0$. The total number of electrons in this region is exactly the number required to make the cell neutral and is equal to the product of the volume of the region and the average density $-\rho_0$. (b) Spherical ion core of radius r_i containing a single nuclear charge Z surrounded by $Q_i^*+B_i$ electrons. (B_i is the total number of bound electrons which defines Q_i^*, the effective number of "free" electrons inside the core.)

plasma prior to averaging over their relative positions. The resulting average-atom potential around a single ion must be totally spherical for a homogeneous isotropic plasma, since no preferred direction is defined. The subsequent distinction, made by the calculation, between the two regions is as follows: In the interior (core) region, the average-atom approximation involves an average over quasispherical electronic states dominated by the field of the central ion, while in the external region $r>r_i$ the average is over configurations (of electrons and ions) that are likely to be far from spherical. One is therefore aware that electron eigenfunctions of the spherically symmetric average-atom Hamiltonian that extend into the exterior region are subject to potentially strong perturbations due to the presence of neighboring ions. Moreover, the model allows the average contribution of those neighboring ions to the potential to be included in a reasonable way.

Denoting the number of electrons within the core by $Q_i^*+B_i$, where B_i is the total number of bound electrons, and the charge of central nucleus by Z_i, the total volume of the cell, which is written as

$$\frac{1}{\hat{\rho}_i}\equiv\frac{4\pi}{3}R_i^3$$

(which defines the ion-sphere radius R_i without necessarily defining an ion sphere), is determined by *charge neutrality condition*

$$Z_i^*-Q_i^*=-\rho_0\frac{4\pi}{3}(R_i^3-r_i^3)\ , \tag{1}$$

where

$$Z_i^*=Z_i-B_i\ .$$

The condition that the cells fill all space is

$$\sum_i\frac{n_i}{\hat{\rho}_i}=1\ . \tag{2}$$

Let the *internal electron polarization parameter* ξ_i^* be defined by

$$\xi_i^*=-\frac{4\pi r_i^3}{3Q_i^*}\rho_0\ , \tag{3}$$

which is the ratio of the number of free electrons within r_i, were they to be unpolarized at a uniform density ρ_0, to the effective number Q_i^*. Equation (1) now gives

$$R_i=\left\{\frac{3}{4\pi}\frac{Z_i^*+(\xi_i^*-1)Q_i^*}{-\rho_0}\right\}^{1/3}\ . \tag{4}$$

Multiplication of both sides of (2) by ρ_0, making use of (4), gives

$$\rho_0=\sum_i n_i\left[\frac{\rho_0}{\hat{\rho}_i}\right]=-\sum_i n_i[Z_i^*+(\xi_i^*-1)Q_i^*]\ . \tag{5}$$

Equations (4) and (5) are generalizations of the standard ion-sphere mixture model equations

$$R_i=\left\{\frac{3}{4\pi}\frac{Z_i^*}{-\rho_0}\right\}^{1/3}\ ,$$

$$\rho_0=-\sum_i n_i Z_i^*\ ,$$

to which they reduce when the free-electron density is constant throughout.

Define the *average* (zero) *plasma potential* to be the ensemble average of the spatial average taken throughout the external regions, each spatial average being taken over a particular plasma configuration. This potential level is associated with the equivalently averaged electron density $-\rho_0$. The chemical potential, referred to this zero potential level, is then reasonably given by the Thomas-Fermi formula[26]

$$\mu=-kTF_{1/2}^{-1}[-\rho_0/c_1(kT)^{3/2}]\ , \tag{6}$$

where F_j^{-1} is the inverse of the function

$$F_j(x)=\int_0^\infty\frac{y^j dy}{1+\exp(x+y)}\ ,$$

while c_1 denotes the physical constant

$$4\pi(2m_e)^{3/2}/h^3\ .$$

In order to quantify the *continuum lowering*,[27–30] one makes a canonical decomposition of the potential into a part due to local charges and a part $V_p(r)$ attributed to the plasma as a whole. The potential $V_p(r)$ is defined to be the average potential due to all charges in $r>r_i$, plus that due to a constant background electron charge density within $r<r_i$. This background electron charge density is chosen to be continuous with the electron charge densi-

ty in the surrounding plasma. This allows one to define a continuous exchange component of the full potential corresponding to $V_p(r)$ and means that the formalism remains implicitly valid for potentials both with and without exchange—in accordance with the general remarks given in Sec. II A. Any alternative definition, which invokes a different constant electron background electron density, yields a decomposition of the exchange potential into components that may be discontinuous at $r=r_i$ (as, for example, in any kind of local-density approximation). These discontinuities render the resulting continuum lowering that one would obtain less meaningful.

The potential $V_p(r)$ can therefore be written

$$V_p(r)=V_>(r)+V_e(r) ,$$

where $V_e(r)$ is the potential due to the background electron charge density within $r<r_i$ and $V_>(r)$ is the average potential due to *all* charges in $r>r_i$. The continuum lowering is defined to be the value of $V_p(0)-V_p(\infty)$, which can be thought of as the shift, due to the plasma, in the binding energy of an arbitrarily deeply bound level (confined near $r=0$) relative to the continuum [assumed to be at $V_p(\infty)$]. It is important to appreciate that there is some degree of arbitrariness in the definition of continuum lowering and that this is largely resolved by convention. A properly formulated self-consistent-field calculation, such as is here being proposed, is independent of the definition of the continuum lowering and does not require any explicit description of it. The continuum lowering is a parameter quantifying one aspect of the effect of the plasma on an ion and is provided as a result of such a calculation. Conversely, the continuum lowering is an incomplete, and therefore approximate, description of the plasma effects and a calculation that seems to depend on it should be regarded with some suspicion.

The results of this section are not dependent on any particular definition of continuum lowering. The potential V_p merely provides a choice of reference potential levels, namely, $V_p(\infty)=V_>(\infty)$, which is the asymptotic *plasma potential,* and $V_p(0)$, which has the role of a *local vacuum*—not to be confused with the real vacuum whose level (relative to μ) defines the *plasma work function.*

In the *internal region* ($r<r_i$), the average electrostatic potential is defined, in the first instance, with respect to the local vacuum $V_p(0)$ as follows:

$$V_{\rm int}(r)=V_<(r)+V_>(r)-V_p(0) ,$$

where $V_<(r)$ denotes the potential due only to the charge distribution within $r<r_i$. In determining the average potential, electric fields, and fields of higher multipolarity, due to external charges (outside r_i) are ignored—these are treated as part of the microfield fluctuation. This leaves $V_>(r)$ being given by only its average monopole component which is constant within $r<r_i$ and therefore equal to $V_>(0)$. Hence the potential $V_{\rm int}$ is provided as a particular solution of Poisson's equation as follows:

$$V_{\rm int}(r)=V_<(r)-V_e(0)$$

$$=\frac{1}{4\pi\epsilon_0}\int_0^{r_i}\frac{\rho(r')}{|\mathbf{r}'-\mathbf{r}|}d\mathbf{r}'-\frac{1}{2\epsilon_0}\rho(r_i)r_i^2 \quad (7a)$$

$$=\frac{1}{4\pi\epsilon_0}\int_0^{r_i}\frac{\rho(r')-\rho(r_i)}{|\mathbf{r}'-\mathbf{r}|}d\mathbf{r}'-\frac{1}{6\epsilon_0}\rho(r_i)r^2 \quad (7b)$$

which is the potential due only to charges within r_i, measured with respect to the potential which would exist at the origin if all the charges within r_i were removed and replaced by electrons at a constant density in equilibrium with the surrounding plasma, while leaving the state of the surrounding plasma unchanged. This potential differs from the plasma potential referred to in Eq. (6) due to the monopole polarization field generated by correlations between the plasma components and the central ion. This is the physical origin of continuum lowering. The potential (7) is provided self-consistently in terms of the total charge density $\rho(r)$, and *vice versa,* through the usual statistical and quantum-mechanical relations of the average-atom model (e.g., Ref. 31).

C. Determination of the core radius r_i

Following Stewart and Pyatt,[28] the core radius is determined by conditions of internal consistency of the model and the requirement that the electric field be a continuous function of position (r). The procedure is therefore to match the derivatives (with respect to r) of the internal and external average electrostatic potentials at $r=r_i$.

Values of the electron density within the core sphere ($r\le r_i$), Z_i^*, and Q_i^* are yielded directly from the quantum-mechanical part of the self-consistent-field calculation. At $r=r_i$, the derivative of the electrostatic potential is given by Gauss's theorem as

$$V'(r_i)=-\frac{Z_i^*-Q_i^*}{4\pi\epsilon_0 r_i^2} ,$$

which, with the aid of (1), becomes

$$V'(r_i)=-\frac{R_i^3-r_i^3}{3\epsilon_0 r_i^2}\rho_0 . \quad (8)$$

For $r\ge r_i$, the potential derivative is taken as being given by

$$V'(r)=-\left[\frac{1}{r}+\frac{1}{D}\right][V(r)-V_p(\infty)] , \quad (9)$$

with the electrostatic potential given in terms of the plasma polarization charge $\rho(r)$ by

$$V(r)=V_p(\infty)-\frac{D^2\rho(r)}{\epsilon_0} , \quad (10)$$

where D is the plasma screening length. Equation (10) can be considered as constituting the definition of D. Equation (9) then applies in the asymptotic region where semiclassical statistical approximations are valid (when D becomes independent of r). The approximation (9 and 10) depends on one of two alternative assumptions: either

that the core extends sufficiently into the asymptotic region (which is true at low to moderate densities) or that the external region ($R_i > r > r_i$), where the validity of the approximation matters, is of negligible extent (which is shown, in Sec. IV, to be the case at very high densities).

The charge density at $r=r_i$ is assumed to be due to electrons alone. These electrons are polarized in the potential $V(r)$, in which case, introducing the characteristic electron screening length d_e, the average electron density at $r=r_i$ can be expressed by

$$\rho(r_i)=\rho_0-\frac{\epsilon_0 V(r_i)}{d_e^2} . \tag{11}$$

Equation (11) here constitutes the definition of d_e and is to be regarded as exact.

Although the instantaneous local ion density is zero at a point in an external region of a typical cell, neighboring ions are not constrained from approaching this point. Indeed the plasma is unpolarized, on average, with respect to such points. Implicit in the underlying cell model of Fig. 4 is that the system of electrons must be capable of maintaining equilibrium contact with an equipotential electron gas at the plasma temperature T, density ρ_0, and chemical potential μ as given by (6). This requires that the "asymptotic" plasma potential $V_p(\infty)$ be synonymous with the "average" plasma potential (zero) defined prior to (6) and is also consistent with the notion (Sec. III) that $V_p(\infty)$ lies at the (true) continuum threshold. Combining (10) and (11), and setting $V_p(\infty)=0$, gives

$$\rho(r_i)=\frac{\rho_0}{1-D^2/d_e^2}=\rho_0\left[\frac{D_I^2}{D^2}\right] ,$$

where

$$\frac{1}{D_I^2}=\frac{1}{D^2}-\frac{1}{d_e^2} . \tag{12}$$

D_I is thus identified as the screening length due to ions alone and is taken as being given by a generalization of the classical Debye form

$$\frac{1}{D_I^2}=\sum_i \frac{1}{D_i^2}, \quad \frac{1}{D_i^2}=\frac{q_i^2 n_i}{\epsilon_0 kT} , \tag{13}$$

where

$$q_i=-\frac{4\pi R_i^3}{3}\rho_0=Z_i^*+(\xi_i^*-1)Q_i^* \tag{14}$$

is the *effective ion charge* (which takes account of the effect of screening by electrons within the ion cores on the interactions between ions). It is assumed that the classical Debye-Hückel theory is applicable to the ions rather than the electrons. Their relatively large mass and (perhaps) charge means that their behavior is more likely to be classical. The approximations represented by Eqs. (9), (12) and (13) are generally regarded as being meaningful only in weak coupling. However, at high densities, in the strong coupling limit, the extent of the region in which the approximations need to be valid becomes vanishingly small. (See Sec. IV.) Justification of Eq. (14) is provided later in Sec. II D.

The total plasma screening length is then given by

$$\frac{1}{D^2}=\frac{\rho(r_i)}{\rho_0}\frac{1}{D_I^2} \Longrightarrow \frac{1}{d_e^2}=\frac{\rho(r_i)-\rho_0}{\rho_0}\frac{1}{D_I^2} , \tag{15}$$

in which d_e is locally dependent on the particular ion species and contains all the quantum-mechanical effects included in the determination of $\rho(r_i)$.

Only two approximations are made in the above. The first involves the assumption that the plasma screening length D is effectively constant for $r \gtrsim r_i$; the second takes the ion screening length, defined by (12), to be given by an appropriate generalization of the classical (Debye-Hückel) formula.

Combining (10) and (15), while recalling that $V_p(\infty)=0$, gives

$$V(r_i)=-\frac{D_I^2\rho_0}{\epsilon_0}\equiv V_s . \tag{16}$$

Note that this is same for all ions—no contact potentials exist between surfaces of different ion cores. This is necessary in view of the presumed approximate uniformity of the potential in the region between the cores. Note that, when $V_s \approx 0$, this yields a muffin-tin–like model of the plasma potential.

Finally, combining Eqs. (8), (9) and (16) gives

$$R_i^3-r_i^3=3D_I^2 r_i\left[1+\frac{r_i}{D}\right]$$
$$=3D_I^2 r_i\left[1+\frac{\alpha_i r_i}{D_I}\right] ,$$

with

$$\alpha_i=\left[\frac{\rho(r_i)}{\rho_0}\right]^{1/2} . \tag{17}$$

Setting $X=r_i/R_i$, $Y=D_I/R_i$, and $\alpha=\alpha_i$ gives

$$X^3+3\alpha X^2 Y+3XY^2-1=0 , \tag{18}$$

which is to be solved for X. The sum of the three roots of this equation is -3α, which is negative definite, while their product is $+1$. The equation therefore possesses either three real roots, one positive and two negative, or two complex (conjugate) roots with negative real parts and one real root which must be positive. In either case the equation always possesses one and only one positive real root—which is the one required.

D. Plasma coupling and effective charges

The parameter Y introduced above is directly related to the *ion coupling parameter* Γ_i according to

$$\left[\frac{R_i}{D_I}\right]^2=\frac{1}{Y^2}=3\Gamma_i . \tag{19}$$

The quantity Γ_i is a measure of the strength of the coupling between the ion i and the surrounding plasma. This can be decomposed into a volumetrically weighted sum

over contributions Γ_i^j from the each of the other ions in the plasma, i.e.,

$$\Gamma_i = \sum_j \frac{n_j}{\hat{\rho}_j} \Gamma_i^j \ , \tag{20}$$

where the *mutual ion-ion coupling parameters* Γ_i^j are defined by

$$\Gamma_i^j = \frac{L_{ij}}{R_i} \ , \tag{21}$$

and where

$$L_{ij} = \frac{q_i q_j}{4\pi\epsilon_0 kT} \tag{22}$$

are the *mutual interaction Landau lengths.*

Combining Eqs. (19)–(22) yields

$$\frac{q_i}{q_j} = \left[\frac{R_i}{R_j} \right]^3 \ , \tag{23}$$

i.e., the effective charge is directly proportional to the volume of the ion cell. Hence we can write

$$q_i = -\gamma \frac{4\pi}{3} R_i^3 \rho_0 \ ,$$

where γ is a constant for the plasma as a whole.

The special case when the electrons are unpolarized and do not give rise to screening yields $\gamma = 1$ and hence $q_i = Z_i^*$. Otherwise, interpreting r_i as the closest distance to which a perturber ion may approach, the minimum screening charge due to the ambient electron polarization seen by the perturbing ion is equal to

$$Q_i^* + \frac{4\pi}{3} r_i^3 \rho_0 \ ,$$

which is the increase, due to polarization, in the number of electrons within r_i. Then, recalling (1), the effective charge is found to be given by

$$q_i = Z_i^* - Q_i^* - \frac{4\pi}{3} r_i^3 \rho_0 = -\frac{4\pi}{3} R_i^3 \rho_0 \ ,$$

which again implies $\gamma = 1$. The reasonableness of the general assignment $\gamma = 1$ is supported by the lack of obvious suitable nontrivial dimensionless constants in the theory in its present form.

Equations (20)–(22) lead to the powerful concept of the *plasma* or *perturber effective charge,*

$$q_p = \sum_j \frac{n_j}{\hat{\rho}_j} q_j \ , \tag{24}$$

which allows many of the properties of the surrounding plasma mixture to be reduced to those of a single component plasma of ions carrying charge q_p. In particular,

$$\Gamma_i = \frac{L_i}{R_i} \ , \tag{25a}$$

where

$$L_i = \frac{q_i q_p}{4\pi\epsilon_0 kT} \tag{25b}$$

is the *generalized Landau length* for species i, and

$$\frac{1}{D_I^2} = -\frac{\rho_0 q_p}{\epsilon_0 kT} \ , \tag{26}$$

which gives directly the ion screening length.

E. Discussion

This then completes the set of equations that are essential to the model. The equations define how the (average) electrostatic potential of an ion should be constructed. Within the sphere $r = r_i$, the potential is determined self-consistently with the aid of (7). In the region $r > r_i$, the potential becomes an average screened type of potential satisfying (9) and (16), e.g., $V_s(r_i/r)\exp[(r_i - r)/D]$, which includes a contribution from other ions. The radius r_i is chosen so that, when these potentials are matched (at r_i), by means of a gauge shift in one of them, the first derivative (electric field) is continuous.

Beyond the surface $r = r_i$, the model allows considerable freedom in how one treats plasma fluctuations and ion-ion collisions. Also, such considerations as how and where the quantum-mechanical boundary conditions should be applied are left open.

The significance of the radius r_i is that electrons within r_i are strongly influenced by the central charge and are only weakly affected by perturbations due to the surrounding plasma. Low-order perturbation theory (e.g., of the Stark effect[41]) will be valid in this region. In particular, it is often reasonable to ignore the possibility of finding perturber ions within r_i. Electrons whose orbitals extend significantly into the region $r > r_i$ are susceptible to strong perturbations due to neighboring ions. Low-order perturbation theory is less likely to be valid since the perturber can approach closer than the central ion and spherical symmetry is strongly broken. This divides the electronic spectrum into, not two (bound and free), but three, not necessarily distinct, regions: (i) deeply bound (weakly perturbed) states, (ii) strongly perturbed bound states which may form a quasicontinuum merging with (iii) the true continuum of nonlocalized states and resonances. A similar sort of picture has been adopted in the plasma model of Rogers.[32,33]

The spherically symmetric potential is just an ensemble average of the microfield taken over many ions. However, in an average-atom treatment, we can consider such an ensemble average as being equivalent to a time average (taken over a suitably long interval) of the properties of a single electron undergoing transitions, in a slow time-dependent potential, between all its accessible states. This is a form of the ergodic hypothesis. What it suggests is that one might be able to treat the plasma fluctuations by means of a *complex potential.* This is an approach, familiar to nuclear physicists, for treating, in a time-independent formalism, states which decay to other channels through processes whose detailed treatment is omitted. The eigenvalues of a complex potential are complex, yielding simultaneously both the energy and

width of a level. The complex eigenvalue approach has already been suggested by More[30,31] as a means of treating continuum resonances. Marrying this with a complex potential will include, in a seemingly practical manner, the all-important effects of plasma perturbations on those resonances and upper bound states.

A suggested form factor for the imaginary part of such a potential is

$$W_i(r)=\frac{\exp(aL_i/R_i)}{(R_i/r)^2\exp(aL_i/r)+\exp(aL_i/R_i)}, \quad a\approx 1 \tag{27}$$

which exhibits reasonable behavior in all the various limits. Such a function can be roughly interpreted as being proportional to the probability that the center of a neighboring ion is closer to the electron at r than the nucleus of the central ion. The strength of the imaginary part will then be related to some mean free path for the electron propagating in the bulk of the plasma.

The theoretical framework also provides direct means of estimating parameters of the microfield. If the electrons are treated as a continuum, then the potential in the plasma region external to all the cores is nonsingular, and it is relatively easy to estimate statistical moments of the microfield, by, for example, assuming each of the ions contributes a screened Coulomb potential, and they are randomly distributed as hard spheres with radii $\sim r_i$. At high Γ, when the r_i become the ion-sphere radii, allowance must be made for the fact that the ion spheres must overlap. This is achieved generally by parametrizing the microfield outside a reduced core, whose radius is taken to be given by $r_i'\simeq r_i(1+\Gamma_i)/(1+\varphi_i\Gamma_i)$ where φ_i is the ratio of ion-sphere diameter to the average separation of the ion centers. This approach permits treatment of nonspherical components of the microfield arising from the discrete distribution of nearest neighbors (see Sec. III B).

III. CONTINUUM LOWERING

A. General formula

The continuum lowering, as defined in Sec. II B is given by

$$\begin{aligned}\Delta V&=V_p(0)-V_p(\infty)\\&\equiv[V_<(r_i)+V_>(r_i)-V_p(\infty)]\\&\quad-[V_<(r_i)+V_>(r_i)-V_p(0)]\\&\equiv V_s-V_{\rm int}(r_i)\ .\end{aligned}$$

In terms of the above, the potentials $V_{\rm int}(r_i)$ and V_s, as defined by (7) and (16), are provided as follows:

$$\begin{aligned}V_{\rm int}(r_i)&=\frac{q_i}{4\pi\epsilon_0 r_i}\left[1-\left[\frac{r_i}{R_i}\right]^3\right]-\frac{1}{2\epsilon_0}\rho(r_i)r_i^2\\&=\frac{q_i}{4\pi\epsilon_0 r_i}\left[1-\left[\frac{r_i}{R_i}\right]^3(1-\tfrac{3}{2}\alpha_i^2)\right],\end{aligned} \tag{28}$$

while from (16),

$$V_s=-\frac{D_I^2\rho_0}{\epsilon_0}=\frac{3q_i}{4\pi\epsilon_0 R_i}\left[\frac{D_I}{R_i}\right]^2 \tag{29a}$$

$$=\frac{1}{\Gamma_i}\frac{q_i}{4\pi\epsilon_0 R_i}=\frac{q_i}{4\pi\epsilon_0 L_i} \tag{29b}$$

$$=\frac{kT}{q_p}\ . \tag{29c}$$

Hence the formula for the continuum lowering is

$$\begin{aligned}\Delta V_i&\equiv V_s-V_{\rm int}(r_i)\\&=\frac{q_i}{4\pi\epsilon_0}\left\{\frac{1}{L_i}-\frac{1}{r_i}\left[1-\left[\frac{r_i}{R_i}\right]^3(1-\tfrac{3}{2}\alpha_i^2)\right]\right\},\end{aligned} \tag{30}$$

which is exact within the context of the model. Figure 5 illustrates the schematic relationship between the various potentials and is helpful in order to understand why $\Delta V_i<0$ [as implied by (30)] corresponds to continuum *lowering*.

Equation (30) is consistent with the simpler result of Stewart and Pyatt to which it reduces in the case of a one-component plasma (OCP) when the i subscripts are dropped (one-component mixture) and α set equal to unity throughout (no electron polarization). Equation (30), on the other hand, applies to a mixture and allows for polarization of the electrons. The change in value of (30), when α_i is set equal to unity, gives the electron polarization contribution to the continuum lowering. (The case $\alpha=1$ applied to a mixture is recognizable as a form of the Steward-Pyatt formula. However, the latter is expressi-

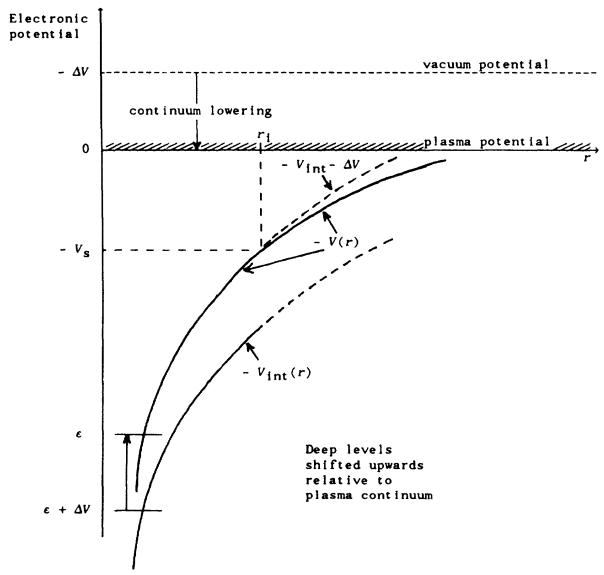

FIG. 5. Shifted and unshifted electronic potentials in the neighborhood of an ion illustrating continuum lowering. Potentials are schematic and are plotted as functions of the radial distance r from the ion center. For additional explanation, see text.

ble in various ways[29] which differ in the way they generalize to mixtures.)

Figures 6(a) and 7(a) illustrate the results of some calculations of the continuum lowering using Eq. (30). These show the various contributions to the continuum lowering for an astrophysical plasma and for a plastic under conditions attainable in a laser experiment. The electronic contribution in these cases is significant. The fluctuation component is the rms microfield calculated as outlined in Sec. II E. The reason for this extra contribution is explained below. Figures 6(b) and 7(b) show the corresponding values of Γ_i and r_i/R_i. Note that, al-

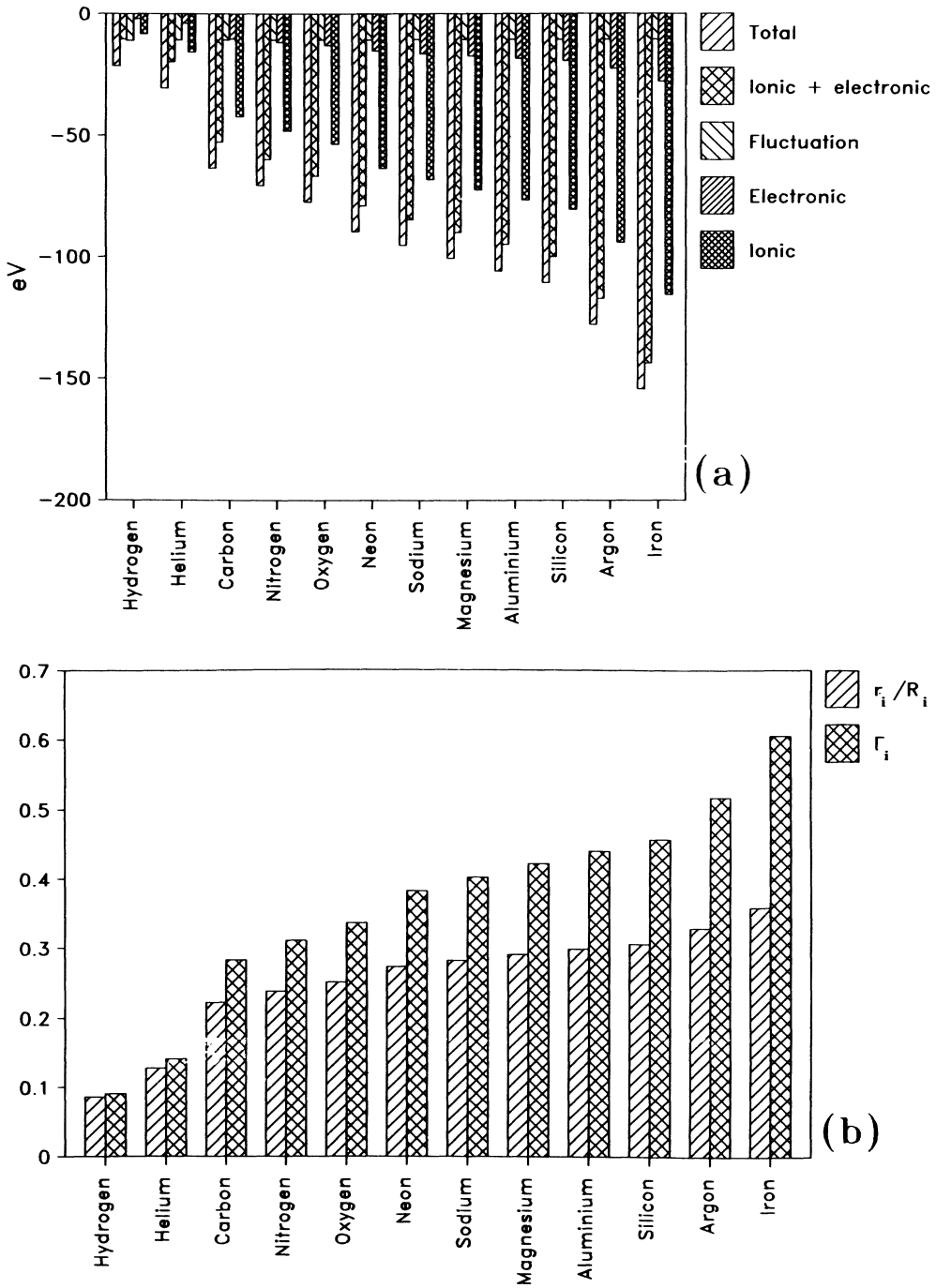

FIG. 6. (a) Continuum lowering, calculated using (30), with an added fluctuation contribution, for an astrophysical plasma characteristic of part of the solar interior (IBEN-XIV mixture, temperature = 300 eV, density = 1.0 g/cm^3). The ionic component of the continuum lowering is given by the Stewart-Pyatt formula in the form of (30) with $\alpha = 1$. The remainder is the electronic contribution. The total continuum lowering is the sum of all three contributions including the fluctuations which are the rms values of the microfield calculated in the annuli $r_i' < r < R_i$ (see Sec. II E). (b) Characteristic values of Γ_i and r_i/R_i for the components of this plasma.

though the plastic is an example of a moderately strongly coupled plasma, the values of r_i work out considerably less than the ion-sphere radii. This is explained by (35), which shows the residual terms to be $O(\Gamma^{-1/2})$.

B. Continuum lowering: general discussion

An occasional misconception about continuum lowering is that it represents an additional correction to the electronic potential within a plasma. This is not so. Any properly formulated self-consistent-field model will always automatically have included the continuum lowering. Equation (30) therefore represents the continuum lowering that is already inherent in the model and does not normally need to be worked out when implementing the model. Proper uses of Eq. (30) include comparisons between different models, estimating where the continuum lies in relation to upper electronic states of an atom and crudely correcting isolated-atom calculations for the presence of the surrounding plasma. However, thermo-

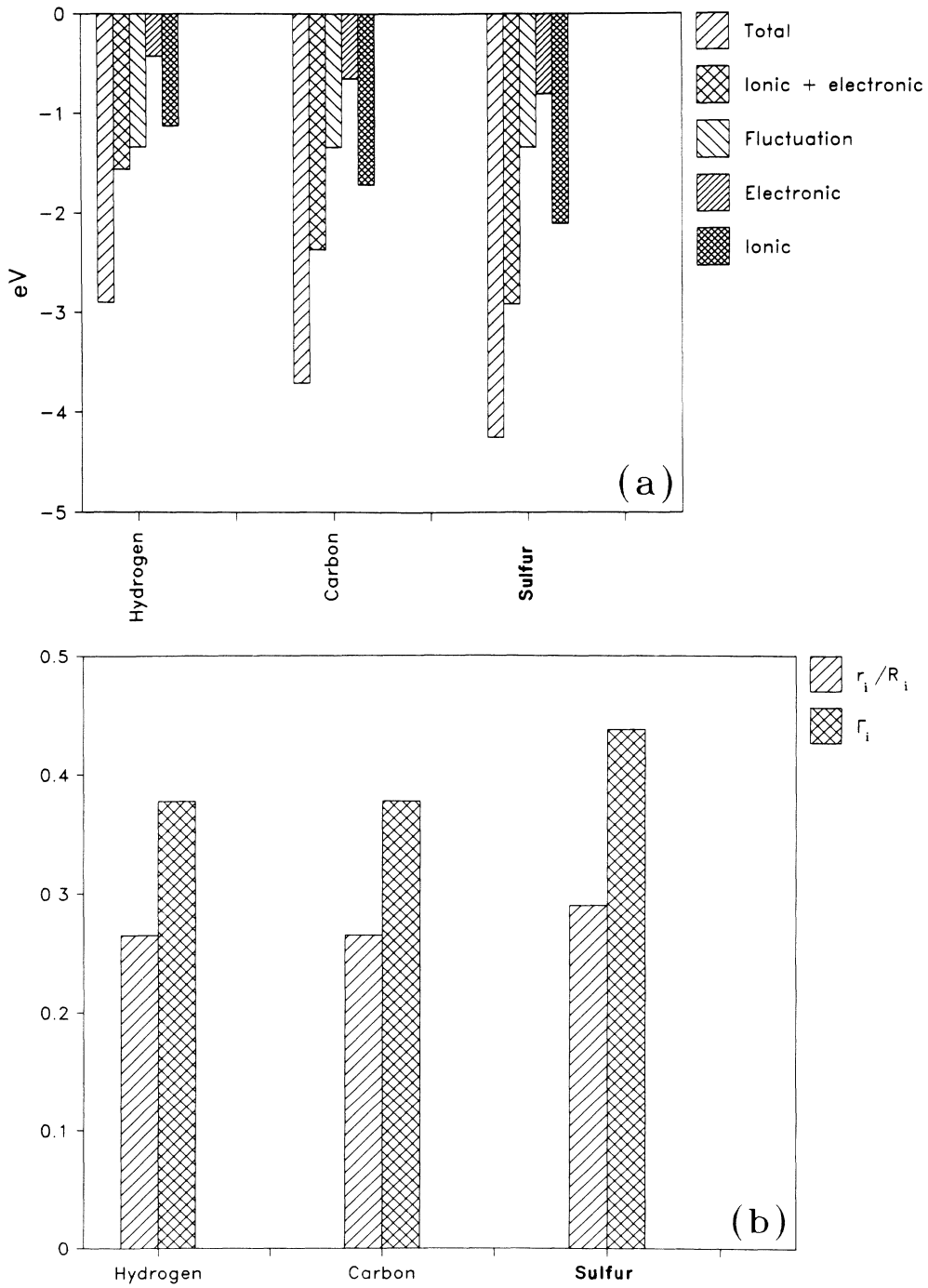

FIG. 7. Same as for Figs. 6(a) and 6(b), but showing continuum lowering and plasma parameters for a laser-heated plastic [PPS (C_6H_7S) at temperature of 5 eV and density of 0.0091 g/cm^3].

dynamic inconsistencies are likely to result if the continuum lowering is introduced in this way.[29,31]

The continuum lowering, as provided by (30), represents an element of the spherically averaged potential. In the presence of a nonspherical component of the microfield, e.g., due to a nearby perturber, the potential barrier surrounding an atom will somewhere be lower than its average, resulting in a further lowering of the apparent ionization threshold.[34,35] Also, microfield broadening of the upper bound states will invariably mean that they merge with the real continuum. These are the arguments for including an additional "fluctuation" term in the continuum lowering of the ionization threshold, as was done in the calculations shown in Figs. 6 and 7.

The continuum lowering derived in Sec. III A is defined in terms of the continuum threshold $[\sim V_p(\infty)]$ associated with a given potential. For atoms in plasmas, the definition may be more usefully expressed in terms of the effect on the energy threshold for photoionization. The first definition is, by virtue of Koopman's theorem, equivalent to the statement that the *change* in the free energy of the system, when an infinitesimal test charge $-\delta q$ is added to the lowest-energy continuum state, is $\Delta V \delta q$, and hence that the minimum energy required to transfer an infinitesimal $-\delta q$ of charge from the level α with eigenvalue ε_α to the continuum is $(\Delta V-\varepsilon_\alpha)\delta q$. If the free energy is expanded as far as quadratic terms in the Taylor series in the atomic configuration, the ionization threshold energy, for the transition

$$N_\alpha, Z^* \rightarrow N_\alpha - 1, Z^* + 1 \ ,$$

is found to be

$$(\Delta V-\varepsilon_\alpha)-\frac{1}{2}\frac{\partial}{\partial N_\alpha}(\Delta V-\varepsilon_\alpha)+\frac{1}{2}\frac{\partial}{\partial Z^*}(\Delta V-\varepsilon_\alpha) \ , \quad (31)$$

in which $\partial\varepsilon_\alpha/\partial Z^* = \partial \Delta V/\partial N_\alpha$. It is evident that, provided that all energies (i.e., eigenvalues, both bound and in the continuum) are referred to the continuum threshold, as defined by the potential for that particular configuration, the continuum lowering is treated implicitly and one does not need to worry about it. In the same vein, a particular consequence of Koopman's theorem is that the energy of an atomic configuration is independent of the number of electrons occupying the level corresponding to the zero energy eigenvalue (i.e., $\partial E/\partial N_0 = \varepsilon_0 \equiv 0$). For a system of *interacting* particles (e.g., electrons) this makes sense if and only if the density of states at $\varepsilon = 0$ is effectively zero for all possible configurations. This leads to the conclusion that the zero energy level common to different configurations within the same plasma corresponds to the continuum threshold $\sim V_p(\infty)$. Note also that the global gauge symmetry is a property of the many-particle system. Global gauge transformations cannot and should not be applied independently to each quasiparticle Hamiltonian. The special significance of the zero energy eigenvalue is a clear indication of the nonarbitrariness of the energy scale to which it is referred.

The continuum lowering is generally *not* the same as the minimum free-energy per electron in the continuum, any more than the free energy of the ion is the sum of the single-particle energy eigenvalues of the occupied bound states. The difference is, of course, due to the Coulomb interaction energy between the electrons, which, for continuum electrons, is always a significant proportion of the total potential energy. Nor, for similar reasons, is it the potential energy per ion pair divided by Z^*—interestingly the electrons matter even in the OCP limit when the free-electron density is assumed constant throughout. This is because the continuum lowering is related to the *change* in the free energy when an electron is added to the continuum. In the extended OCP model,[36–39] there is an effect due to the correlation between the ion's charge and its separation from neighboring ions due to increased Coulomb repulsion when an electron is removed and added to the background. In the ion-sphere model, this pair correlation is neatly treated through the expansion of the ion sphere. Because, in reality, the ions are free to move within the plasma, this leads to the need to distinguish between the continuum lowering and the specific free energy (per electron per ion pair). Failure to do so has resulted in some confusion in one or two places in the literature, not the least in Stewart and Pyatt's original paper. This has led to misapprehension concerning their formula. The situation is that Stewart and Pyatt's paper[28] describes, not one, but two different models. The first leads to their celebrated formula, which, as will be shown, is correct. The second, a numerical model which attempts to be more sophisticated, makes the error alluded to. The outcome is that, if one attempts to calculate the ion free energy from the incorrect formula $\Delta F_c = \frac{1}{2} Z^* \Delta V$, which ignores the pair-correlation effect mentioned above, taking ΔV as given by the first formula, one obtains the result that $\Delta F_c = -\frac{3}{4}(Z^* e)^2/(4\pi\epsilon_0 R)$, in the large-$\Gamma$ limit, instead of the correct result given below. This deficiency was pointed out by More[29] and has resulted in the misapprehension that the original formula is itself defective.

To put the record straight, in the OCP ion-sphere model of More and Zimmerman,[40] the continuum contribution to the free energy of an ion is (assuming $Z^* \gg 1$)

$$\Delta F_c = -\frac{9}{10}\frac{(Z^* e)^2}{4\pi\epsilon_0 R} \ ,$$

with

$$R^3 = \frac{3Z^*}{4\pi\rho_e} \ ,$$

where ρ_e is the average free-electron density in the plasma [cf. Eq. (14) above]. This yields the continuum-lowering as

$$\Delta V = \frac{\partial \Delta F_c}{\partial Z^*} = -\frac{3}{2}\frac{Z^* e^2}{4\pi\epsilon_0 R} \ ,$$

in complete agreement with the Stewart-Pyatt formula [cf. Eq. (36a) below], while the first of these equations agrees, to within about $\frac{1}{2}\%$, with the extended-OCP formula of DeWitt,[39] in the limit of $\Gamma \sim \infty$. This is quite remarkable agreement considering the relative simplicity of the ion-sphere model.

IV. SPECIAL CASES

A. Solution in the weak-coupling limit (ideal plasma)

Solving Eq. (18) for a weakly coupled ion ($\Gamma_i \ll 1$) yields r_i as the generalized Landau length [Eqs. (25)],

$$r_i \sim \Gamma_i R_i [1-\Gamma_i (3\Gamma_i)^{1/2}] \sim \Gamma_i R_i = L_i \ , \tag{32}$$

which is expressly much less that R_i. Note the corollary

$$\frac{1}{r_i} \sim \frac{1}{L_i} + \frac{1}{D_I} \ . \tag{33}$$

The average potential beyond r_i is the screened Coulomb (Debye-Hückel) potential. However, this is also the region in which pressure broadening effects due to the microfield of neighboring ion perturbers are likely to be important.[41–46]

In the weak-coupling limit ($\Gamma_i \ll 1$), Eq. (30) reduces, by virtue of (33), to

$$\Delta V_i = -\frac{q_i}{4\pi\epsilon_0 D_I}[1+O(\Gamma_i^3)] \ , \tag{34}$$

which gives the continuum lowering in a form resembling the usual Debye-Hückel result, e.g., Refs. 29, 30, and 47–50. Note the appearance of the effective charge q_i in place of Z_i^*.

B. Solution in the strong-coupling limit

For a strongly coupled ion ($\Gamma_i \gg 1$), the limiting solution of (18) is

$$r_i \sim R_i [1-\alpha_i/(3\Gamma_i)^{1/2}] \sim R_i \ , \tag{35}$$

from which we see that the model reduces to the standard spherical ion-cell model. The region $r_i < r < R_i$, in which the potential is assumed to be given by a Debye-Hückel type of screened potential, becomes vanishingly small, so that the question of the validity of introducing such a potential form in this limit does not pose any serious difficulty. Also, the account taken of weakening of ion-ion interactions by electron screening ameliorates any (apparently slight) discrepancy between the ion-sphere model and the extended-OCP model at very high Γ's. This might arise because the ion-sphere model does not include a proper treatment of the ion-ion correlations. Electron screening tends to reduce Γ and the longer-range correlations between ions, while the electronic screening effects may be the more important.

In the strong-coupling limit ($\Gamma_i \gg 1$), the continuum lowering (30) becomes

$$\Delta V_i = -\frac{3}{2}\frac{q_i \alpha_i^2}{4\pi\epsilon_0 R_i}[1+O(\Gamma_i^{-1/2})] \ , \tag{36a}$$

which resembles the ion-sphere result.[29–31,40] Substituting for $q_i\alpha_i^2$ from (14) and (17) yields an alternative form of (36a)

$$\Delta V_i = -\frac{\rho(r_i)R_i^2}{2\epsilon_0}[1+O(\Gamma_i^{-1/2})] \ , \tag{36b}$$

which relates the result to the electron density at the ion-sphere–ion-core surface.

The results expressed by Eqs. (36) and (34) generalize the previously known formulas to mixtures while taking account of electron polarization.

V. SUMMARY

The new generalized ion-cell model of an atomic plasma described here overcomes many of the defects of the standard models listed in Sec. I. Although this model contains the other models as its limits, the extra degrees of freedom introduced into the treatment obviate the inadequacies. The scope of the model extends to any mixture of elementary ions, which may be particular ionization states or average-atom representations of different elements, in local thermodynamic equilibrium. (Non-LTE generalizations of the model appear feasible.)

The model remains a single-atom cell model even at low densities, but copes with the problem of strongly overlapping ion spheres in this regime by allowing typical cells to be nonspherical. In this picture, the ion-sphere radius enters only as a parametrization of the density. In the average-atom approximation, one has taken an average over all possible configurations (including nonspherical "terms"). The resulting potential is always spherically symmetric. However the model now recognizes the presence of "other ions" in the region outside the core. As will all cell models, the extent of the physical system addressed by the model is unambiguous and allows rigorous application of statistical mechanics and thermodynamics.

The spherical core within each cell defines the region in which a conventional spherical average-atom approximation has strong validity, i.e., in which perturbations due to fluctuations of the surrounding plasma microfield are generally weak. Within such regions, one can perform self-consistent quantum mechanics with real potentials. Where wave functions extend significantly into the exterior plasma region, it is necessary to take account of the plasma microfield which is both nonspherical and statistical in nature. In the exterior region, the electrons are treated using the Thomas-Fermi statistical model. Whereas this is likely to be a good approximation in the majority of cases, it is not a necessary feature of the basic model. Enhanced statistical models[18–25] may be used in place of the Thomas-Fermi model, if the latter is thought inadequate.

In the high-density (strong-coupling) limit, the model reduces to the standard spherical ion-cell model. However, it is noted that this limit is attained only for very large values of the coupling parameter Γ_i.

In the low-density (weak-coupling) limit, the model defines the core region to be a Landau sphere beyond which the potential is allowed to take the form of the Debye-Hückel polarization potential. The model will accommodate a complex potential to account for perturber fluctuations at distances beyond the core radius.

The model copes with all intermediate regimes, including plasmas comprising mixtures of components characterized by both small and large values of Γ. A useful

concept for use in treating individual components of a mixture is that of the effective plasma or perturber charge which characterizes the effects of the surrounding plasma.

One of the principal features of the model is that it consistently takes account of polarization of the electrons and the consequent weakening of the effective interaction between the ions. This polarization is given in terms of the quantum-mechanical solution for the electrons within the spherical core. The model thus obviates one of the principal deficiencies of the OCP model, while its own deficiencies in relation to the OCP have, in the past, been overstated.

The model yields explicit formulas for the continuum lowering, and plasma work function (which is taken to be the volume average of the continuum lowering). In the strong- and weak-coupling limits, respectively, the formulas resemble the ion-sphere and Debye-Hückel formulas for an OCP. The new formulas improve on the OCP by treating electron polarization. In a self-consistent numerical implementation, the continuum lowering is implicit.

A virtue of the new model is its essential simplicity. It is hardly any more difficult to implement than the standard SIC algorithm which it generalizes. Moreover, it retains considerable flexibility concerning details of the calculation that remain beyond its scope. Indeed, the model often permits better treatments of such details due to its adopting a more general paradigm. For example, improved treatments of fluctuations, both of the plasma microfield and the charge state of the ion, become possible within the context of an average-atom cell model. In the latter instance, this is helped by the distinction that is made, even at high densities, between the core and the average-ion cell. While the average-ion cell remains neutral (by definition), the core charge can fluctuate. The cores may therefore be treated as a grand canonical ensemble. When treating the microfield fluctuations and their effects,[41–46] the model permits one to identify easily which electronic states are susceptible to strong (nonlinear) perturbations from the surrounding plasma and which may be amenable to simpler weak perturbation treatments. A simple approach to estimating statistical moments of the microfield itself is suggested.

In conclusion, the new model offers greater generality and wider applicability than either the SIC or PCS types of model (which it incorporates in its limits and therefore replaces) and provides a powerful extension to the average-atom statistical description of LTE plasma.

ACKNOWLEDGMENTS

The author would like to thank Daryl Landeg and Colin Smith for their helpful comments on the preparation of the manuscript.

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