

# Reduced formulation and efficient algorithm for the determination of equilibrium composition and partition functions of ideal and nonideal complex plasma mixtures

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The system of coupled nonlinear Saha equations supplemented by electroneutrality and conservation of nuclei for complex plasma mixtures is reformulated into a reduced form, which allows the development of an efficient numerical algorithm to solve the set of nonlinear equations. The efficient algorithm is based on the solution of an equivalent single transcendental equation. Nonideality corrections have been taken into consideration in terms of depression of ionization potentials and truncated partition functions. Implementing this simple efficient methodology simplifies the problem and considerably reduces the computational effort needed to compute the detailed plasma composition for different cases. The algorithm is analytically known to be safe, fast, and efficient. It also shows no numerical instabilities, no convergence problems, and no accuracy limitations or lack of change problems, which have been reported in the literature. A nontrivial sample problem has been worked in detail showing the usefulness of the method for applied and industrial plasma physicists. Effects of the nonideality corrections and the exclusion of excited states are quantified and presented. A criterion for the validity of the assumption of local thermodynamic equilibrium is applied to the results from the sample problem to show the region of the temperature-density phase space over which the assumption is valid.

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## I. INTRODUCTION

Precise and reliable information about thermodynamic, transport, and radiative properties of complex plasma mixtures in a wide range of temperatures and densities is needed for the solution of many scientific and technological problems arising in industrial plasma engineering and high-energy density physics. However, the quantitative investigation of these properties necessitates information about the detailed plasma composition at a specified temperature and a fixed number density of heavy particles. Particle densities of plasma components (charged particles as well as neutral particles) are required for the calculation of plasma kinetic pressure, internal energy, enthalpy, sound speed, adiabatic exponent, as well as transport properties such as electric conductivity, viscosity, thermal conductivity, opacities, and ion stopping power. Gas mixtures in plasma torches, mixtures in plasma display panels [1,2], shielding gas mixtures in laser welding of metals [3], dense-plasma lasers, plasmas generated from Teflon, polyethylene, and Lexan polycarbonate in electrothermal-chemical plasma guns [4–6] are a few examples of plasma mixtures for which computing the detailed plasma composition is required for the development, functioning, and optimization of these devices. If the assumption of local thermodynamic equilibrium (LTE) is applicable, the distribution of atoms and their ionization products (ions and electrons) obeys the Saha equation [7]. Taking into account the lowering of ionization potentials due to nonideal effects [8–11], the Saha equation—for a single elemental species plasma—can be written as

$$\frac{n_{r+1}n_e}{n_r} = 2 \frac{U_{r+1}}{U_r} \left[ \frac{2\pi m_e K_B T}{h^2} \right]^{3/2} \exp\left(-\frac{I_r^{\text{eff}}}{K_B T}\right),$$

$$r = 0, 1, \dots, (Z-1), \quad (1)$$

where  $n_e$  is the number density of free electrons,  $n_r$  is the number density of all  $r$ -fold ionized atoms,  $U_r$  is the state-dependent partition function of  $r$ -fold ionized atoms,  $m_e$  is the mass of an electron,  $h$  is Planck's constant, and  $I_r^{\text{eff}} = I_r - \Delta I_r$  is the effective ionization energy for the ionization process  $r \rightarrow (r+1)$ ,  $\Delta I_r$  is the lowering of ionization potential. Equation (1) can be derived from thermodynamic principles through the minimization of Gibbs free energy, and therefore it can be considered a mass action law for the process of ionization. The system of Saha equations (1), supplemented by the condition of electro-neutrality,

$$\sum_{i=1}^Z in_i = n_e, \quad (2)$$

and requiring a constant number of heavy particles (conservation of nuclei in the ionization and recombination processes),

$$\sum_{r=0}^Z n_r = n_h, \quad (3)$$

is sufficient for the calculation of the composition of a plasma generated from a single chemical species. However, plasmas generated from compound materials or from mixtures of gases are more complex than plasmas generated from a single chemical species. For these complex plasmas, the equations for different chemical species are linked through the electron number density and the common temperature. According to Glowacki [3], “the case of the monatomic gas mixture is more complicated and has not been presented in the literature previously.” In Ref. [3] the case of an ideal mixture of two monatomic gases has been treated where the technique by Trayner and Glowacki [12] has been

used to solve the equations. However, concerns about numerical stability were reported; this is of course in addition to the accuracy limitations (lack of change problems) of the algorithm used and which are reported in Ref. [12]. Numerical stability concerns and problems were even reported for the simplest case of solving a single Saha equation (with unity as the maximum ionization state) coupled to an energy equation when a Newton-Raphson technique was used [13]. In this paper we clear the complexity of the problem and show a simple, safe and stable, fast, and accurate solution of this problem. The method depends on the reduction of the set of nonlinear equations into a simple form (an equivalent single transcendental equation), which requires minimal numerical work to be solved.

Although it is common knowledge that safety in obtaining convergence and numerical stability are crucial for such a problem, it may be useful to clarify why accuracy and computational time are also of interest. Regardless of the well-known fact that better numerical techniques (e.g., more accurate) should replace worse ones if they need the same computational efforts or less, accuracy and computational time are of interest for the following.

(i) It is obvious that any procedure does not allow the computations of the populations of different species if their population does not exceed the accuracy of the procedure. Therefore, in a weakly ionized gas, if the population of any species does not exceed the accuracy, the method fails.

(ii) Time derivative of the ionization state may be also required in many applications (see, for example, Ref. [14]). If the increment in time  $dt$  is small enough such that the change in the ionization is comparable to the accuracy, the derivative term may assume the opposite sign which may be catastrophic and seriously impose restrictions on the solution of the physical problem under consideration. Recalling that time derivative is just an example and the argument applies to the derivative with respect to any other parameter it becomes clear that accuracy may be crucial in the calculation of ionization equilibrium.

(iii) Finally, calculating the ionization equilibrium of the plasma is not the ultimate goal. It is needed for the calculation of thermodynamic functions, transport, and optical properties. In a typical simple self-consistent hydrodynamic simulation one needs to calculate the ionization equilibrium several millions of times. Time saving in the calculation of ionization equilibrium, however small it is, leads to a huge time savings in the overall time needed for the computations.

Hence improvements in terms of solution accuracy and computational time, in addition to safety in obtaining convergence and stability of the solution, are also valuable and needed.

## II. A REDUCED FORMULATION FOR PLASMA MIXTURES

It is assumed that all chemical compounds and polyatomic molecules are fully dissociated, i.e., all chemical reactions other than ionization and recombination are not included. The plasma mixture in this case is effectively a mixture of inert gases and hence the plasma composition can be com-

pletely described by the set of nonlinear Saha equations with the conservation of electric charge and conservation of nuclei. This is obviously the case for diatomic molecules if the plasma temperature is several thousand degrees. However, and because of the weaker bonds, polyatomic molecules begin dissociation at even lower temperatures [9]. If one refers to the chemical species in the mixture by the subscript  $j$  and the total number of the elemental species by  $J$  then from the requirement of *constant number of heavy particles* (conservation of nuclei) one has

$$\sum_{r=0}^{Z_j} n_{r,j} = n_{h,j}$$

and

$$\sum_{j=1}^J n_{h,j} = n_H,$$

where  $n_{h,j}$  is the number density of heavy particles (nuclei) of elemental species  $j$ ,  $n_H$  is the total number density of heavy particles of all elemental species in the mixture, and  $Z_j$  is the atomic number (or the maximum allowed ionization stage) of elemental species  $j$ . Dividing the above two equations by  $n_H$  one gets

$$\sum_{r=0}^{Z_j} \alpha_{r,j} = c_j, \quad (4a)$$

where  $\alpha_{r,j} = n_{r,j}/n_H$  and  $c_j = n_{h,j}/n_H$  are the molar fractions of the  $r$ -fold ionized ions of the elemental species  $j$  and the total molar fraction of the elemental species  $j$ , respectively. Summing over all elemental species yields

$$\sum_{j=1}^J c_j = 1. \quad (4b)$$

Similarly, the condition of *quasineutrality* (conservation of electric charge) gives

$$\sum_{i=1}^{Z_j} i n_{i,j} = n_{e,j}$$

with

$$\sum_{j=1}^J n_{e,j} = n_e,$$

where  $n_{i,j}$  is the number density of  $i$ -fold ionized ions of the elemental species  $j$ ,  $n_{e,j}$  is the number density of free electrons introduced to the system by ionizing the atoms/ions of

the elemental species  $j$ , and  $n_e$  is the total number density of free electrons. In principle, free electrons can take any energy and, they should be considered *indistinguishable*. Accordingly, the subscript  $j$  in the term  $n_{e,j}$  must not be misread as a sort, or quality distinguisher, but rather as a quantity or share assigner for different sources of free electrons (elemental species). Dividing the above two equations by  $n_H$  one gets

$$\sum_{i=1}^{Z_j} i \alpha_{i,j} = \bar{Z}_{e,j} \quad (5a)$$

and

$$\sum_{j=1}^J \bar{Z}_{e,j} = Z_{av}, \quad (5b)$$

where  $\bar{Z}_{e,j} = n_{e,j}/n_H$  is the contribution of the free electrons liberated from the elemental species  $j$  to the average charge per heavy particle  $Z_{av}$ , defined as  $Z_{av} = n_e/n_H$ . One can express the set of nonlinear *Saha equations* in terms of the proportions  $\alpha$ 's, average charge state  $Z_{av}$ , and the total number density of heavy particles  $n_H$  such that

$$\frac{n_{r+1,j} n_e}{n_{r,j}} = f_{r+1,j}(T, n_e, \dots)$$

or

$$\frac{\alpha_{r+1,j} Z_{av} n_H}{\alpha_{r,j}} = f_{r+1,j}(T, n_e, \dots),$$

where the Saha coefficients  $f_{r+1,j}$ 's have been written in a general form to account for any possible formulas for the lowering of ionization potentials. For ideal plasmas the Saha coefficients are functions of the temperature only. The above equations give the following recurrence relation:

$$\alpha_{r+1,j} = \frac{\alpha_{r,j}}{Z_{av} n_H} f_{r+1,j}(T, n_e, \dots). \quad (6)$$

Substituting from Eq. (6) into Eq. (5a) one gets

$$\sum_{i=1}^{Z_j} i \frac{\alpha_{i-1,j}}{(Z_{av} n_H)^i} f_{i,j}(T, n_e, \dots) = \bar{Z}_{e,j}.$$

Upon successive use of the recurrence relation (6) into the above equation one can obtain

$$\alpha_{0,j} = \frac{\bar{Z}_{e,j}}{\sum_{i=1}^{Z_j} \frac{i}{(Z_{av} n_H)^i} \prod_{m=1}^i f_{m,j}(T, n_e, \dots)}. \quad (7)$$

Substituting from Eq. (7) and relation (6) into Eq. (4a) gives

$$\begin{aligned} c_j &= \sum_{r=0}^{Z_j} \alpha_{r,j} \\ &= \alpha_{0,j} \left( 1 + \sum_{i=1}^{Z_j} \frac{\prod_{m=1}^i f_{m,j}(T, n_e, \dots)}{(Z_{av} n_H)^i} \right) \\ &= \bar{Z}_{e,j} \left[ \left( 1 + \sum_{i=1}^{Z_j} \frac{\prod_{m=1}^i f_{m,j}(T, n_e, \dots)}{(Z_{av} n_H)^i} \right) / \sum_{i=1}^{Z_j} \frac{i}{(Z_{av} n_H)^i} \prod_{m=1}^i f_{m,j}(T, n_e, \dots) \right] \end{aligned}$$

from which

$$\bar{Z}_{e,j} = c_j \times \left[ \sum_{i=1}^{Z_j} \frac{i}{(Z_{av} n_H)^i} \prod_{m=1}^i f_{m,j}(T, n_e, \dots) / \left( 1 + \sum_{i=1}^{Z_j} \frac{\prod_{m=1}^i f_{m,j}(T, n_e, \dots)}{(Z_{av} n_H)^i} \right) \right] \quad (8)$$

and substituting from Eq. (8) into Eq. (5b) one gets

$$Z_{av} = \sum_{j=1}^J c_j \times \left[ \sum_{i=1}^{Z_j} \frac{i}{(Z_{av} n_H)^i} \prod_{m=1}^i f_{m,j}(T, n_e, \dots) / \left( 1 + \sum_{i=1}^{Z_j} \frac{\prod_{m=1}^i f_{m,j}(T, n_e, \dots)}{(Z_{av} n_H)^i} \right) \right]. \quad (9)$$

Equations (6)–(9) constitute a reduced formulation of the set of nonlinear Saha equations subjected to the condition of quasineutrality and the requirement of constant number of heavy particles. For the case of a pure single elemental species ( $J=1$ ), Eqs. (9) and (8) become identical with  $Z_{av} = \bar{Z}_{e,j}$ .

The solution of the set of equations in its current form is very simple and can be performed safely and accurately as shown below. Since the Saha coefficients  $f_{m,j}$ s include the state-dependent partition functions  $U_{r,j}$ , it is appropriate to discuss the computations of the internal partition functions before presenting the method of solution of this system of Eqs. (6)–(9).

### III. CALCULATION OF THE INTERNAL PARTITION FUNCTION

The total internal partition function  $U_r$  (or the sum over all states) is a dimensionless quantity, which for an isolated atom/ion can be formally evaluated according to the equation

$$U_r = \sum_{n=1}^{\infty} g_{r,n} \exp\left(-\frac{E_{r,n}}{K_B T}\right), \quad (10)$$

where  $E_{r,n}$  is the  $n$ th excitation energy of species  $r$  (counted from the ground state) and  $g_{r,n}$  is its statistical weight. In the calculation of the internal partition function, all equilibrium populations (ground/excited states) have to be included. Equation (10), in which  $g_{r,n} = 2J_n + 1$  where  $J_n$  is the total angular momentum, implies that the populations of the excited states follow a Boltzmann distribution. For an isolated (free) atom/ion,  $U_r$  diverges and finite values are obtained only when interaction with the environment are accounted for in order to truncate the sum. Recalling that in a plasma environment, the ionization energies are reduced such that excitation states with very high  $n$  do not exist, and the partition function actually converges. The summation in Eq. (10) is thus limited to a maximum of  $n = n^*$ , which corresponds to a maximum energy  $E_{n^*}$ . In the computations of the partition function the summation is performed over all the available spectroscopic data [15] for the excitation energies and terminated at energy level  $E_{n^*}$ , which is related to the effective ionization energy  $I_r^{\text{eff}}$  by the relation  $E_{n^*} \leq I_r^{\text{eff}} = I_r - \Delta I_r$ . This means that the partition function is a function of  $T$  and  $\Delta I$  ( $T, \rho$ ) just like the exponential term of the Saha coefficients. This means that the solution technique of the Saha equations is the same whether one includes the excited states in the calculation of the partition functions or just by considering the ground states only. However, the results may differ and the impact of such an approximation on the computations of ionization equilibrium needs to be investigated and quantified.

### IV. METHOD OF SOLUTION

The method of solution of the set of Eqs. (6)–(9) depends on the formula used for the lowering of ionization potentials. Practically, one can face the following cases.

(i) *Ideal plasma* with no lowering of ionization potential.

In such a case, the Saha coefficients  $f$ 's are functions of the temperature only and Eq. (9) is a transcendental equation in  $Z_{av}$ , the solution of which is eminently simple. Many software packages include solvers for transcendental equations or algorithms for finding the zeros of a function. In addition, efficient algorithms that use a combination of bisection, secant, and inverse quadratic interpolation methods can also be found in Ref. [16]. For cases in which one is only interested in determining the average ionization state,  $Z_{av}$ , the solution of the transcendental equation (9) will suffice. However, if the interest extends to the determination of the detailed composition of different elemental species and different ionization stages, simple direct back-substitution into Eqs. (8), (7), and (6) will be required to determine the detailed composition. The algorithm is simply articulated in the following steps:

(1) solve the transcendental equation (9) for  $Z_{av}$ ;

(2) substitute in Eq. (8) to determine  $\bar{Z}_{e,j}$  for the elements of interest;

(3) substitute for  $Z_{av}$ , and  $\bar{Z}_{e,j}$  in Eq. (7) to calculate  $\alpha_{0,j}$  (proportions of neutral atoms) for the elements of interest; and

(4) use the recurrence relation (6) to calculate all the  $\alpha_{r+1,j}$ 's of interest.

(ii) *Nonideal plasma* with expressions for the lowering of ionization potentials  $\Delta I_{r,j}$  that can be expressed explicitly in terms of  $Z_{av}$  and other known quantities such as  $n_H$ , for example. In this case also, Eq. (9) is a transcendental equation in  $Z_{av}$ . The method of solution is then identical to the case of ideal plasmas. Examples of such models for the lowering of ionization potentials can be found elsewhere [10].

It may be useful at this point to highlight some of the benefits and advantages gained (for these two cases) by reformulating the equations into this reduced form. For these two cases the solution of the problem is reduced to the trivial problem of solving a transcendental equation. Hereby, for these two cases, the problem of evaluating the plasma composition is shown to be effectively a one-dimensional nonlinear problem with only one independent variable,  $Z_{av}$  (namely, finding the root of a function). According to Ref. [16], “simultaneous solution of equations in  $N$  dimensions is much more difficult than finding roots in the one-dimensional case. The principal difference between one and many dimensions is that, in one dimension, it is possible to bracket or ‘trap’ a root between bracketing values, and then hunt it down like a rabbit. In multi-dimensions, you can never be sure that the root is there at all until you have found it.” Moreover, in principle, the zero of a transcendental equation can be determined to any degree of accuracy on the expense of the computational time (i.e., no accuracy limitations). Therefore accuracy of computations of detailed plasma composition will be only dictated by machine characteristics.

(iii) *Nonideal plasma* and  $\Delta I_{r,j}$  cannot be expressed explicitly in terms of  $Z_{av}$  and known quantities but rather in terms of a common parameter (such as the Debye length  $\lambda_D$ ), that depends on the individual  $\alpha$ 's. The model proposed by Griem

[8] is an example of such a case. In this model the lowering of ionization potentials is given by

$$\Delta I_{r,j} = \frac{(r+1)e^2}{4\pi\epsilon_0\lambda_D}, \quad (11)$$

with  $\lambda_D$  defined as

$$\lambda_D = \left[ \epsilon_0 K_B T / e^2 \left( n_e + \sum_{j=1}^J \sum_{r=0}^{Z_j} r^2 n_{r,j} \right) \right]^{1/2}. \quad (12)$$

A similar, widely used model proposed by Ebeling *et al.* [11] gives the lowering of ionization potentials as

$$\Delta I_{r,j} = \frac{(r+1)e^2}{4\pi\epsilon_0(\lambda_D + \Lambda_B/8)}, \quad (13)$$

where  $\Lambda_B = h/\sqrt{2\pi m_e K_B T}$  is the de Broglie wavelength and  $\lambda_D$  is expressed as in Eq. (12). With a bit of analysis and insight, the solution in this case can also be obtained with simplicity and to any desired accuracy. The fact that Eq. (9) can be simply and accurately solved for any specified value of  $\lambda_D$  makes it, effectively, equivalent to an algebraic expression of the form

$$Z_{av} = \bar{f}_1(\lambda_D). \quad (14)$$

In the same time, the definition of  $\lambda_D$  in Eq. (12) can be rewritten as

$$\lambda_D - f_2(\lambda_D, Z_{av}) = 0. \quad (15)$$

Now, upon substitution from Eq. (14) into Eq. (15) one gets

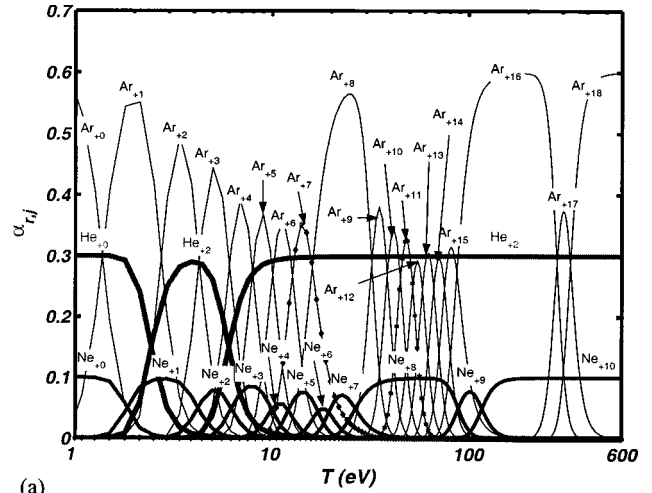
$$\lambda_D - f_2(\lambda_D, \bar{f}_1(\lambda_D)) = 0 \quad (16)$$

which is a transcendental equation in  $\lambda_D$ . The bar over  $f_1$  refers to the numerical nature of the function  $f_1$ . Even for case (iii), in which  $\Delta I_{r,j}$  cannot be expressed explicitly in terms of  $Z_{av}$  and known quantities but rather in terms of the common parameter  $\lambda_D$ , the present analysis shows that the problem of evaluating the plasma composition for a complex mixture is effectively a one-dimensional nonlinear problem (or simply finding the root of a function) with one independent variable  $\lambda_D$ . Therefore, even for such a case, the plasma composition can be determined with simplicity and to any desired accuracy. It is interesting that solving Eq. (16) simultaneously gives the values of  $\lambda_D$ ,  $Z_{av}$ ,  $\bar{Z}_{e,j}$ 's,  $U_{r,j}$ 's, and  $\alpha_{r,j}$ 's and therefore it represents the whole algorithm. In the following section a sample problem that represents this case is worked in detail.

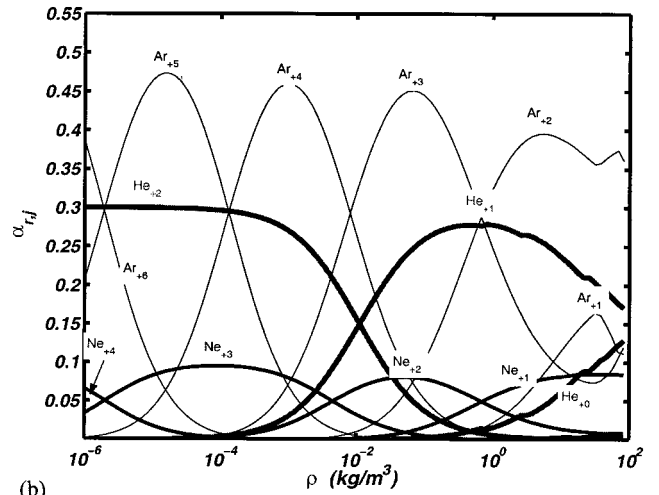
A model in which the nonideal plasma corrections  $\Delta I_{r,j}$ 's can neither be expressed explicitly in terms of  $Z_{av}$  and known quantities nor in terms of a common parameter that depends on the individual  $\alpha$ 's is not known to the author at the present time.

### V. A SAMPLE PROBLEM

The current methodology has been applied to compute the composition of many complex plasma mixtures. A helium-neon-argon plasma mixture is arbitrarily selected to work



(a)



(b)

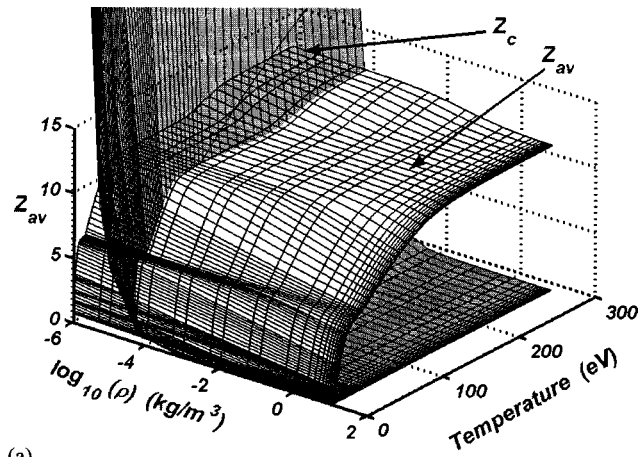
FIG. 1. (a) Temperature dependence of the detailed equilibrium composition of a 0.1-kg/m<sup>3</sup> [He(0.3):Ne(0.1):Ar(0.6)] plasma mixture. (b) Density dependence of equilibrium composition of a 5-eV [He(0.3):Ne(0.1):Ar(0.6)] plasma mixture.

this problem. However, a concentration of [He(0.3) : Ne(0.1) : Ar(0.6)] is chosen to give better readability of the crowded figures presented in this section. Necessary atomic data and excitation and ionization energies have been taken from Ref. [15]. A comprehensive set of energy levels (more than 3000 for the three elements) has been used in the computations of the partition functions. The model for nonideality correction (lowering of ionization potential) proposed by Ebeling *et al.* [11], which represents case (iii) as shown above, is used to run this sample problem. For this case, all nonlinearity of the problem is reduced into the single transcendental equation (16) which can be solved with simplicity to the machine accuracy for  $\lambda_D$ ,  $Z_{av}$ , and  $\alpha_{r,j}$ 's in the same time.

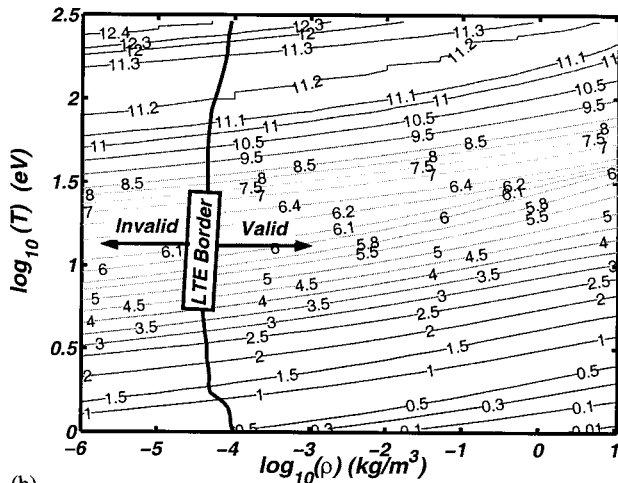
### A. Results

Figure 1(a) shows the temperature dependence of the molar fractions of different ionic species in a 0.1-kg/m<sup>3</sup> He/Ne/Ar plasma mixture with the composition shown in the





(a)

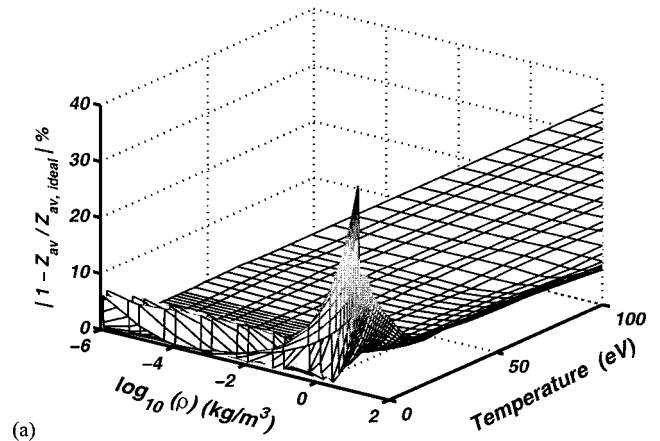


(b)

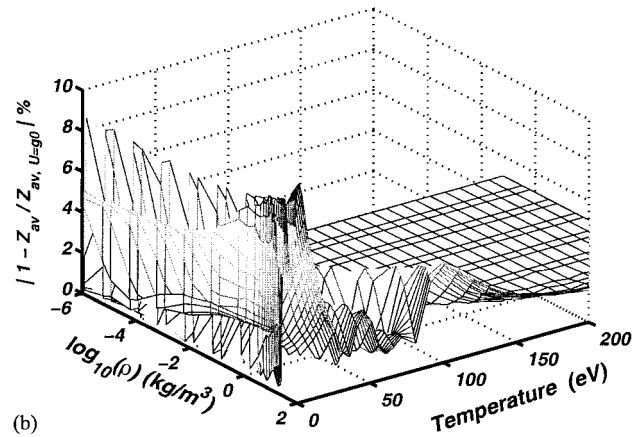
FIG. 2. (a) Surface plots of  $Z_{av}$  and  $Z_c$  for [He(0.3):Ne(0.1):Ar(0.6)] plasma mixture. (b) Contours of constant  $Z_{av}$  and the boundary for the validity of the LTE assumption for [He(0.3):Ne(0.1):Ar(0.6)] plasma mixture.

figure. As the temperature increases, the molar fractions of neutral species (He, Ne, and Ar) decrease monotonically as a result of the progressive ionization. With further increase of the temperature, higher ionized ionic species appear at the expense of lower-fold ionized species. Figure 1(b) shows the detailed plasma composition for a 5-eV plasma (for the same mixture) at different densities.

An average nuclear charge can be approximately assigned to this plasma mixture and the critical (minimum) electron number density required for LTE can be determined as a function of temperature. The criterion given by Fujimoto and McWhirter [17] is adopted and applied for the present computations. For each density, a critical value for the average ionization state  $Z_c$  can be calculated by dividing the critical electron number density by the corresponding  $n_H$  and one can verify the validity of the LTE assumption by comparing both of  $Z_{av}$  and  $Z_c$  as shown in Fig. 2(a). Figure 2(b) is a useful representation of the calculated ionization data where contours of  $Z_{av}$  are presented as functions of  $T$  and  $\rho$ . The logarithmic axes scales have been used to cover a wide range of temperatures and densities. As shown in the figure the



(a)



(b)

FIG. 3. (a) Nonideality effects on the computations of  $Z_{av}$  for [He(0.3):Ne(0.1):Ar(0.6)] plasma mixture. (b) Effect of excluding the excited states from the computations of the partition function on the computations of  $Z_{av}$  for [He(0.3):Ne(0.1):Ar(0.6)] plasma mixture.

LTE assumption can be considered for He(0.3)/Ne(0.1)/Ar(0.6) plasma mixture with densities  $> 10^{-4} \text{ kg/m}^3$ . From both parts it can be seen that at very high temperatures the average ionization state approaches its expected theoretical limiting value for a fully stripped plasma, i.e.,  $Z_{av} = 12.4$ .

Figure 3(a) shows a surface plot of the nonideality effect on the computations of the average ionization state. As it is very clear from the figure, the nonideality corrections (lowering of ionization potentials) have a significant effect at low temperatures and relatively high density. Figure 3(b) shows a surface plot of the percentage relative difference between the average ionization state calculated including the excitation states in the computations of the partition functions and those calculated approximating the partition functions to the statistical weights of the ground states. A maximum percentage difference less than 10% can be seen from the figure. Higher difference values are also relevant to the region of low temperature and/or high density. Therefore it can be concluded that considering the nonideality effects and detailed computation of the partition functions becomes important for the region of low temperature and/or high density in the  $\rho$ - $T$  phase space.

### B. Discussion

The results presented above have some interesting remarks that need some discussion. For example, a peculiar behavior is to be seen in Fig. 2(b) where a large “gap” opens in the region between 11.2 and 11.3 for  $Z_{av}$  in the  $\rho$ - $T$  plane. This gap occurs at temperatures where both of the He and Ne atoms are mostly fully stripped with the remaining species ( $Ar_{+16}$ ) having the heliumlike stable configuration [see Fig. 1(a)]. Accordingly, this gap is expected to occur in the vicinity of  $Z_{av} = (0.3) \times 2 + (0.1) \times 10 + (0.6) \times 16 = 11.2$ , which is in agreement with Fig. 2(b). Due to its stable configuration, the curve for  $F_{+16}$  shows a wide distribution function of temperature [see Fig. 1(a)]. Similar behavior can be also recognized with  $Ne_{+8}$  for the aforementioned reason (He-like configuration). Another important point is in regard to the effect of excluding the excited states on the computations of  $Z_{av}$ . As shown in Fig. 3(b), the effect is considerable in the region of high density and/or low temperature. There is no significant effect in the region where the density is low and/or where the temperature is high enough. This behavior can be understood if we bear in mind that the effect of including the excited states on the computations of  $Z_{av}$ , depends on both of the values of the partition functions and, *more importantly*, on the population of the bound excited states. At high temperatures and low densities, recombination is weak and high ionization states occur with the result that the population of the bound/excited states is low. Accordingly, excluding the excited states in this region of the  $\rho$ - $T$  phase space does not have a recognized impact on the computations of  $Z_{av}$ . On the other hand, for low temperature and/or high densities, ionization is inhibited by recombination and atoms and ions become more fully excited before they ionize resulting in a dense population of bound/excited states. Under these circumstances, the exclusion of the ex-

cited states in this region of the  $\rho$ - $T$  phase space will considerably impact the computations as shown in Fig. 3(b).

### VI. CONCLUSIONS

The system of coupled nonlinear Saha equations supplemented by electroneutrality and conservation of nuclei for complex plasma mixtures is reformulated into an equivalent reduced form, which allows the development of an efficient numerical algorithm to solve the set of nonlinear equations. Nonideality corrections have been taken into consideration in terms of depression of ionization potentials and truncated partition functions. In most practical cases the solution of the set of  $1 + \sum_j Z_{max,j}$  coupled nonlinear equations in  $1 + \sum_j Z_{max,j}$  unknowns is reduced to the simple problem of solving a single transcendental equation. Implementing this simple efficient methodology simplifies the problem and considerably reduces the computational effort needed to compute the detailed plasma composition for different cases. The method is analytically known to be safe, fast and efficient. It also shows no numerical instabilities, no convergence problems and no accuracy limitations or lack of change problems, which have been reported in the literature. The present analysis and methodology supports the belief that computational success crucially depends on analysis and insight rather than numerics. A nontrivial sample problem has been worked in detail showing the usefulness of the method for applied and industrial plasma physicists.

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